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STRUCTURE FILE UPDATES: 13 APR 2004 HIGHEST RN 675103-21-6 DICTIONARY FILE UPDATES: 13 APR 2004 HIGHEST RN 675103-21-6

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=> d sta que 147 L25 STR

VAR G1=AK/4/6/10/14/19/26/28/30/32/34/37/41/44 NODE ATTRIBUTES:

NSPEC IS RC AT 1
CONNECT IS M1 RC AT 1
CONNECT IS M1 RC AT 19
CONNECT IS M1 RC AT 48
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

pt //

RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 46

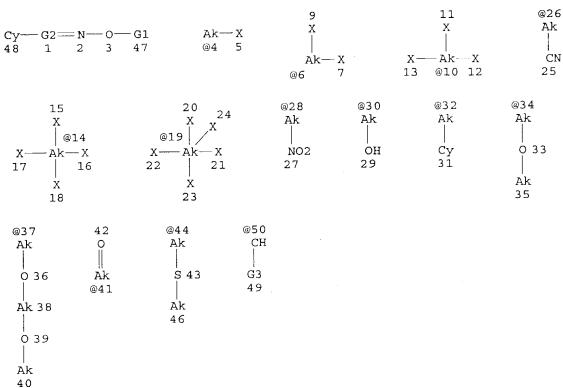
STEREO ATTRIBUTES: NONE

L27

46016 SEA FILE=REGISTRY CSS FUL L25

L36

STR



VAR G1=AK/4/6/10/14/19/26/28/30/32/34/37/41/44 VAR G2=CH/50VAR G3=CN/X/AK/4/6/10/14/19 NODE ATTRIBUTES: CONNECT IS M1 RC AT 19 CONNECT IS M1 RC AT 48 DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

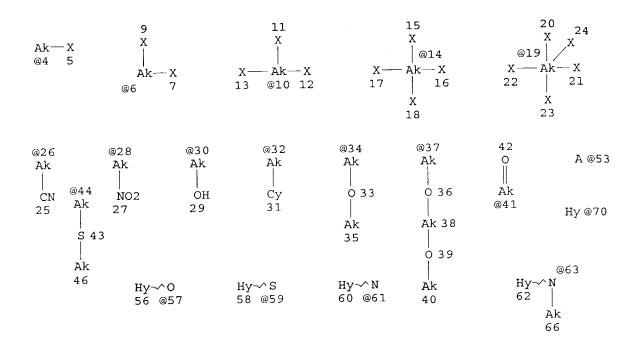
RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 48

STEREO ATTRIBUTES: NONE

4398 SEA FILE=REGISTRY SUB=L27 CSS FUL L36 L38

L45 STR $G2 \sim G3 \sim G4 \sim Cy - C = N - O - G1$ 51 50 49 48 1 2 3 47



VAR G1=AK/4/6/10/14/19/26/28/30/32/34/37/41/44

ну-- сн2-- о

67 68

VAR G2=70/57/59/61/63/69/55

REP G3 = (0-1) AK

Ну∽ Ну 54 @55

REP G4 = (0-2) 53

NODE ATTRIBUTES:

IS RC ΑT 1 NSPEC 1 CONNECT IS M1 RC AT 48 RC AT CONNECT IS M1 RC AT 53 CONNECT IS M1 RC AT 54 CONNECT IS M1 RC AT 55 CONNECT IS M1 CONNECT IS M1 RC AT 56 RC AT 58 CONNECT IS M1 RC AT 60 CONNECT IS M1 62 RC AT CONNECT IS M1 RC AT 67 CONNECT IS M1 RC AT 70 CONNECT IS M1 DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 65

STEREO ATTRIBUTES: NONE

1307 SEA FILE=REGISTRY SUB=L38 CSS FUL L45

100.0% PROCESSED 4398 ITERATIONS SEARCH TIME: 00.00.01

1307 ANSWERS

(FILE 'HOME' ENTERED AT 08:23:26 ON 15 APR 2004) SET COST OFF

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FILE 'HCAPLUS' ENTERED AT 08:23:44 ON 15 APR 2004
               1 S WO2000-AU680/AP, PRN
L1
                 E WU W/AU
             366 S E3,E28,E29
L2
                 E WU WEN/AU
             102 S E3,E115
L3
                 E WU WENY/AU
               2 S E6
L4
                 E WATSON K/AU
L5
             272 S E3-E18
                 E WATSON KEITH /AU
             134 S E3-E14
L6
                 E MCCONNELL D/AU
             116 S E3-E8, E13, E14
L7
                 E MC CONNELL D/AU
                 E JIN B/AU
             307 S E3-E14
L8
              21 S E81
L9
                  E KRIPPNER G/AU
              21 S E3-E5
L10
                  E BIOTA/PA,CS
              54 S E3-E37
L11
                  SEL RN L1
      FILE 'REGISTRY' ENTERED AT 08:26:50 ON 15 APR 2004
             197 S E1-E197
L12
              23 S L12 NOT OXIME
T.13
               5 S L13 AND (C20H22CLN5O2 OR C18H21N3O3 OR C22H29N3O4S OR C21H27N
L14
              18 S L13 NOT L14
L15
             179 S L12 NOT L15
L16
               2 S L16 AND (C9H11NO2 OR C7H7NO)
L17
             177 S L16 NOT L17
L18
                  SAV L18 CRANE018/A
                  STR
L19
L20
                0 S L19 CSS SAM
                0 S L19 SAM
L21
                  STR L19
L22
                0 S L22 CSS SAM
L23
                0 S L22 SAM
L24
                  STR L22
L25
               50 S L25 CSS SAM
L26
           46016 S L25 CSS FUL
L27
                                               LYZ = Fry 69, Chare

XZ forma signoich

AR

No alecant hits

L31 = Cylicants
                  SAV TEMP L27 CRANE018A/A
              174 S L12 AND L27
L28
                3 S L18 NOT L28
L29
                2 S L29 NOT C16H21NO2
L30
              176 S L28, L30
L31
                  STR L25
L32
                0 S L32 CSS SAM SUB=L27
L33
                  STR L32
L34
                0 S L34 CSS SAM SUB=L27
L35
                  STR L34
L36
               50 S L36 CSS SAM SUB=L27
 T<sub>1</sub>3.7
             4398 S L36 CSS FUL SUB=L27
 L38
                  SAV TEMP L38 CRANE018B/A
                  STR L36
 L39
                  STR L39
 L40
                1 S L40 CSS SAM SUB=L27
 L41
               18 S L40 CSS FUL SUB=L27
 L42
```

```
SAV L42 TEMP CRANE018C/A
L43
                STR L25
              0 S L43 FUL SUB=L42
T.44
                 SAV L44 CRANE018D/A
                 STR L25
T<sub>1</sub>45
             50 S L45 CSS SAM SUB=L38
L46
           1307 S L45 CSS FUL SUB=L38
L47
                 SAV L47 TEMP CRANE018E/A
           1142 S L47 NOT L12
L48
     FILE 'HCAPLUS' ENTERED AT 09:21:59 ON 15 APR 2004
L49
              2 S L31
              2 S L49 AND L1-L11
L50
            391 S L48
L51
            363 S L51 AND (PD<=19990618 OR PRY<=19990618 OR AY<=19990618)
L52
                 E RHINOVIR/CT
                 E E4+ALL
           1306 S E7, E6+NT
L53
                 E E5+ALL
            736 S E6,E5
1.54
          10479 S E5+NT
L55
              0 S L52 AND L53
L56
               0 S L52 AND L54
L57
               0 S L52 AND L55
L58
              1 S L51 AND L53-L55
L59
              1 S L51 AND (?RHINOVIR? OR ?PICORNAVIR?)
L60
              2 S L50, L59, L60
1.61
              41 S L52 AND (?VIRUS? OR ?VIRAL? OR ?VIRUC?)
L62
                 E ANTIVIRAL/CT
                 E E5+ALL
          43597 S E10, E11, E9+NT
L63
          10840 S E20
L64
                 E VIRUS INFECTION/CT
                 E VIRA INFECTION/CT
                 E VIRAL INFECTION/CT
                 E E3+ALL
           10840 S E2
L65
L66
              42 S L51 AND L63-L65
                                                  LSI, LSZ = only

a good o hits for L79

which real on Structure
              38 S L52 AND L66
L67
              42 S L62, L67
L68
                 E VIRUS, ANIMAL/CT
          112431 S E3
L69
                 E E3+ALL
                 E E2+ALL
            7236 S E5,E3
L70
             10 S L52 AND L69-L70
              42 S L68, L71
              0 S L72 AND (ENTEROVIR? OR COXSA
L73
             225 S L48 (L) (THU OR BAC OR DMA O
L74
                                                   Agreences for There in L87
              34 S L74 AND L72
L75
              20 S L75 NOT P/DT
L76
              14 S L75 NOT L76
L77
              8 S L72 NOT L75
L78
              42 S L72 AND L74-L78
L79
                 SEL HIT RN
                                                   LG(= applicants
      FILE 'REGISTRY' ENTERED AT 09:52:05 ON 15
              75 S E1-E75
L80
               4 S L80 AND C12H14N6O2
L81
               3 S L80 AND (C17H14FN30 OR C17H15N3OS OR C18H15N3O2S)
L82
      FILE 'HCAPLUS' ENTERED AT 10:03:37 ON 15 APR 2004
```

6 S L81 OR L82

L83

s and love

L84 4 S L83 AND (PY<=1999 OR PRY<=1999 OR AY<=1999)

L85 2 S L84 AND L53-L55,L63-L65,L69,L70

L86 3 S L84 AND (?VIRUS? OR ?VIRAL? OR ?VIRUC? OR ENTEROVIR? OR COXSA

L87 4 S L84-L86

FILE 'REGISTRY' ENTERED AT 10:06:16 ON 15 APR 2004

=> fil hcaplus FILE 'HCAPLUS' ENTERED AT 10:06:36 ON 15 APR 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 15 Apr 2004 VOL 140 ISS 16 FILE LAST UPDATED: 14 Apr 2004 (20040414/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d all tot 161 hitstr

L61 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2003:463807 HCAPLUS

DN 139:173249

ED Entered STN: 18 Jun 2003

TI An Orally Bioavailable Oxime Ether Capsid Binder with Potent Activity against Human Rhinovirus

AU Watson, Keith G.; Brown, Renee N.; Cameron, Rachel; Chalmers, David-K.; Hamilton, Stephanie; Jin, Betty; Krippner, Guy Y.; Luttick, Angela; McConnell, Darryl B.; Reece, Phillip A.; Ryan, Jane; Stanislawski, Pauline C.; Tucker, Simon P.; Wu, Wen-Yang; Barnard, Dale L.; Sidwell, Robert W.

Biota Chemistry Laboratory, School of Chemistry, Monash University,

Victoria, 3800, Australia
SO Journal of Medicinal Chemistry (2003), 46(15), 3181-3184
CODEN: JMCMAR; ISSN: 0022-2623

PB American Chemical Society

DT Journal

LA English

CC 1-5 (Pharmacology)

from

$$Me \xrightarrow{N-N} N \xrightarrow{ \left\{ -CH_2 \right\}_2} O \xrightarrow{ NOEt } H$$

CS

GΙ

ST IT

TT

TT

IT

IT

TT

TT

RE

The Et oxime ether (I) rhinovirus (HRV) using a CPE based assay. was found to have outstanding anti-HRV activity (median IC50 4.75 ng/mL), and unlike the equivalent Et ester compound, Pirodavir, it has good oral bioavailability, making it a promising development candidate. I illustrates that an oxime ether group can act as a metabolically stable bioisostere for an ester functionality. oral bioavailable oxime ether antiviral human Rhinovirus Virion structure (capsid; orally bioavailable oxime ether capsid binder with potent activity against human Rhinovirus) Antiviral agents Bioavailability Human Human rhinovirus (orally bioavailable oxime ether capsid binder with potent activity against human Rhinovirus) 577792-16-6P RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (orally bioavailable oxime ether capsid binder with potent activity against human Rhinovirus) 124437-42-9P 124437-50-9P 314062-82-3P 124436-59-5P, Pirodavir 314062-85-6P 314062-87-8P 314062-88-9P 314062-89-0P 314062-90-3P 314062-91-4P 577792-12-2P **577792-13-3P** 577792-11-1P 314062-93-6P 577792-17-7P 577792-15-5P 577792-14-4P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (orally bioavailable oxime ether capsid binder with potent activity against human Rhinovirus) 622-26-4, 120-47-8, Ethyl 4-hydroxybenzoate 141-30-0 4-Piperidineethanol 1121-79-5 RL: RCT (Reactant); RACT (Reactant or reagent) (orally bioavailable oxime ether capsid binder with potent activity against human Rhinovirus) 124438-66-0P 124438-73-9P 124438-52-4P 124438-51-3P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (orally bioavailable oxime ether capsid binder with potent activity against human Rhinovirus) 577792-10-0P RL: SPN (Synthetic preparation); PREP (Preparation) (orally bioavailable oxime ether capsid binder with potent activity against human Rhinovirus) THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT 27 (1) Andries, K; Antimicrob Agents Chemother 1992, V36, P100 HCAPLUS (2) Andries, K; Antiviral Res 1991, V16, P213 HCAPLUS (3) Andries, K; The Search for Antiviral Drugs 1993, P179 (4) Anon; WO 0078746 2001 HCAPLUS (5) Arruda, E; Antiviral Chemotherapy 1995, P321 (6) Bromidge, S; J Med Chem 1997, V40, P4265 HCAPLUS (7) Burger, A; Prog Drug Res 1991, V37, P287 HCAPLUS (8) Diana, G; Antiviral Chem Chemother 1997, V8, P401 HCAPLUS (9) Diana, G; J Comput-Aided Mol Design 1993, V7, P325 HCAPLUS (10) Dragovich, P; J Med Chem 1999, V42, P1213 HCAPLUS (11) Giranda, V; Acta Crystallogr 1995, VD51, P496 (12) Giranda, V; Structure-Based Drug Design 1997, P487 (13) Hadfield, A; Proc Natl Acad Sci U S A 1999, V96, P14730 HCAPLUS

(14) Hayden, F; Abstracts of 40th Interscience Conference on Antimicrobial

Agents and Chemotherapy, Abstract 1161 2000

- (15) Hayden, F; Antimicrob Agents Chemother 1992, V36, P727 MEDLINE
- (16) Hayden, F; Antimicrob Agents Chemother 1995, V39, P290 HCAPLUS
- (17) Hayden, F; www.viropharma.com/healthcare/clinical.html
- (18) Karabatsos, G; Tetrahedron 1967, V23, P1079 HCAPLUS
- (19) Lipinski, C; Annu Rep Med Chem 1986, V21, P283 HCAPLUS
- (20) Makela, M; J Clin Microbiol 1998, V36, P539 MEDLINE
- (21) McKinlay, M; Annu Rev Microbiol 1992, V46, P635 HCAPLUS
- (22) Oren, D; J Mol Biol 1996, V259, P120 HCAPLUS
- (23) Patani, G; Chem Rev 1996, V96, P3147 HCAPLUS
- (24) Sidwell, R; Appl Microbiol 1976, V22, P797
- (25) Stokbroekx, R; US 4992433 1990 HCAPLUS
- (26) Tebbe, M; J Med Chem 1997, V40, P3937 HCAPLUS
- (27) Turner, R; Pediatr Ann 1998, V27, P790 MEDLINE
- IT 577792-16-6P

RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(orally bioavailable oxime ether capsid binder with potent activity against human Rhinovirus)

RN 577792-16-6 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime, [C(E)]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

IT 314062-82-3P 314062-85-6P 314062-87-8P

314062-88-9P 314062-89-0P 314062-90-3P

314062-91-4P 314062-93-6P 577792-13-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(orally bioavailable oxime ether capsid binder with potent activity against human Rhinovirus)

RN 314062-82-3 HCAPLUS

CN Ethanone, 1-[4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]phenyl], O-ethyloxime (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} N-\text{ OEt} \\ \parallel \\ C-\text{ Me} \end{array}$$

RN 314062-85-6 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)

Me
$$N$$
 N CH_2-CH_2-O CH_3-OMe

RN 314062-87-8 HCAPLUS CN Ethanone, 1-[4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]phenyl]-, O-methyloxime (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{N-OMe} \\ \parallel \\ \text{C-Me} \\ \end{array}$$

RN 314062-88-9 HCAPLUS
CN 1-Propanone, 1-[4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]phenyl]-, O-methyloxime (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{N-OMe} \\ \parallel \\ \text{C-Et} \end{array}$$

RN 314062-89-0 HCAPLUS CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-propyloxime (9CI) (CA INDEX NAME)

C1
$$N \longrightarrow CH_2 - CH_2 - O$$
 $CH = N - OPr - n$

RN 314062-90-3 HCAPLUS CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-(1-methylethyl)oxime (9CI) (CA INDEX NAME)

$$C1$$
 N
 N
 CH_2-CH_2-O
 CH_3-O

314062-91-4 HCAPLUS RN

Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-, CNO-2-propenyloxime (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{C1} & \text{N} & \text{CH}_2\text{-CH}_$$

314062-93-6 HCAPLUS RN

Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-, CN O-(phenylmethyl)oxime (9CI) (CA INDEX NAME)

$$C1$$
 N
 CH_2-CH_2-O
 CH_2-Ph

577792-13-3 HCAPLUS RN

Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-, CNO-ethyloxime, [C(E)]- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

HCAPLUS COPYRIGHT 2004 ACS on STN **6**F 2 L61 ANSWER 2

2000:911241 HCAPLUS AN

DN 134:71606

Entered STN: 29 Dec 2000 ED

Preparation of (heterocyclyl)alkoxy benzaldehyde oximes as antiviral ΤI agents

Wu, Wen-Yang; Watson, Keith; Mcconnell, Darryl TN ; Jin, Betty; Krippner, Guy

Biota Scientific Management Pty. Ltd., Australia PΑ

PCT Int. Appl., 84 pp. SO

CODEN: PIXXD2

DTPatent

English LA

IC ICM C07D401-04 C07D403-04; C07D261-08; C07D237-10; C07D417-04; A61K031-501; A61K031-42; A61K031-50; A61K031-4453; A61P031-12

28-17 (Heterocyclic Compounds (More Than One Hetero Atom)) CCSection cross-reference(s): 1, 10

FAN.CNT 1

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DATE
                                           APPLICATION NO.
                           DATE
                      KIND
     PATENT NO.
                      _ _ _ -
                            _____
     _____
                                                            20000616
                            20001228
                                           WO 2000-AU689
                     A1
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             CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GE, GH, GM, HR, HU,
             ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU,
             LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD,
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             CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
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     EP 1187827
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             IE, SI, LT, LV, FI, RO
                            20030121
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     JP 2003502418
                            19990618
PRAI AU 1999-1054
                       Α
                            20000616 <--
     WO 2000-AU680
                       W
OS
     MARPAT 134:71606
GΙ
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$$C1 - N - N$$

$$CH_2 = 0$$

$$H$$

$$H$$

$$II$$

The title compds. Het-A-Alk-W-Ar-C(X2):NOX1 [I; Het = (un)substituted 5-6 membered monocyclic heterocyclic radical, (un)substituted 9-10 membered bicyclic heterocyclic radical; A = 0, S, NH, etc.; Alk = alkylene, a bond; W = 0, S, OCH2, etc.; Ar = (un)substituted 5-6 membered monocyclic aryl, (un)substituted 9-10 membered bicyclic aryl; X1 = alkyl, alkenyl, alkynyl, etc.; X2 = H, CN, F, etc.], useful in the treatment picornavirus infections in mammals, were prepared Thus, reacting 4-{2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy}benzaldehyde in EtOH with a solution of EtONH2 in H2O afforded 44% O-ethyloxime II. Biol. data (activity against, e.g., HRV-1A, HRV-2, HRV-14, enterovirus 70, Coxsackie A21) for compds. I was given.

benzaldehyde oxime heterocyclylalkoxy prepn antiviral picornavirus; rhinovirus antiviral benzaldehyde oxime heterocyclylalkoxy prepn; enterovirus antiviral benzaldehyde oxime heterocyclylalkoxy prepn; coxsackievirus antiviral benzaldehyde oxime heterocyclylalkoxy prepn

IT Antiviral agents

Enterovirus

Human coxsackievirus A21

Human rhinovirus 14

Human rhinovirus 2

Picornaviridae

(preparation of (heterocyclyl)alkoxy benzaldehyde oximes as antiviral agents)

IT Human rhinovirus

(type 1A; preparation of (heterocyclyl)alkoxy benzaldehyde oximes as antiviral agents)

IT 314062-80-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of (heterocyclyl)alkoxy benzaldehyde oximes as antiviral agents)

IT 314062-79-8P 314062-81-2P 314062-82-3P

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314062-83-4P 314062-84-5P 314062-85-6P
314062-86-7P 314062-87-8P 314062-88-9P
314062-89-0P 314062-90-3P 314062-91-4P
314062-92-5P 314062-93-6P 314062-94-7P
314062-95-8P 314062-96-9P 314062-97-0P
314062-98-1P 314063-00-8P 314063-01-9P
314063-02-0P 314063-04-2P 314063-05-3P
314063-06-4P 314063-07-5P 314063-08-6P
314063-09-7P 314063-10-0P 314063-11-1P
314063-12-2P 314063-13-3P 314063-15-5P
314063-16-6P 314063-17-7P 314063-18-8P
314063-19-9P 314063-20-2P 314063-22-4P
314063-23-5P 314063-25-7P 314063-26-8P
314063-27-9P 314063-28-0P 314063-32-6P
314063-33-7P 314063-35-9P 314063-36-0P
314063-37-1P 314063-38-2P 314063-39-3P
314063-40-6P 314063-41-7P 314063-42-8P
314063-43-9P 314063-44-0P 314063-45-1P
314063-46-2P 314063-47-3P 314063-48-4P
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314063-55-3P 314063-57-5P 314063-59-7P
314063-60-0P 314063-61-1P 314063-64-4P
314063-66-6P 314063-67-7P 314063-68-8P
314063-69-9P 314063-70-2P 314063-71-3P
314063-72-4P 314063-73-5P 314063-74-6P
314063-75-7P 314063-76-8P 314063-77-9P
314063-78-0P 314063-79-1P 314063-80-4P
314063-81-5P 314063-82-6P 314063-83-7P
314063-84-8P 314063-85-9P 314063-86-0P
314063-87-1P 314063-89-3P 314063-90-6P
314063-91-7P 314063-95-1P 314063-96-2P
314063-98-4P 314063-99-5P 314064-01-2P
314064-03-4P 314064-04-5P 314064-05-6P
314064-06-7P 314064-07-8P 314064-08-9P
314064-09-0P 314064-13-6P 314064-14-7P
314064-15-8P 314064-16-9P 314064-17-0P
314064-18-1P 314064-19-2P 314064-20-5P
314064-21-6P 314064-22-7P 314064-23-8P
314064-24-9P 314064-25-0P 314064-26-1P
314064-27-2P 314064-28-3P 314064-29-4P
314064-30-7P 314064-31-8P 314064-32-9P
314064-33-0P 314064-34-1P 314064-36-3P
314064-40-9P 314064-44-3P 314064-46-5P
314064-47-6P 314064-48-7P 314064-49-8P
314064-50-1P 314064-51-2P 314064-52-3P
314064-53-4P 314064-54-5P 314064-55-6P
314064-56-7P 314064-57-8P 314064-58-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
   (preparation of (heterocyclyl) alkoxy benzaldehyde oximes as antiviral
   agents)
314062-99-2 314063-03-1 314063-14-4
314063-21-3 314063-24-6 314063-29-1
314063-30-4 314063-31-5 314063-34-8
314063-49-5 314063-50-8 314063-54-2
314063-56-4 314063-58-6 314063-62-2
314063-63-3 314063-65-5 314063-88-2
314063-92-8 314063-93-9 314063-94-0
314063-97-3 314064-00-1 314064-02-3
314064-10-3 314064-11-4 314064-12-5
314064-35-2 314064-38-5 314064-42-1
314255-60-2
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IT

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(preparation of (heterocyclyl)alkoxy benzaldehyde oximes as antiviral agents)

IT 123-08-0, 4-Hydroxybenzaldehyde 141-30-0 622-26-4, 4-Piperidineethanol 932-90-1, Benzaldehyde oxime 2508-29-4, 5-Amino-1-pentanol 41731-52-6, Ethyl 2-chloro-4-thiazolecarboxylate 54044-79-0, 2-Bromo-5-methyl-1,3,4-thiadiazole 124437-50-9 124438-51-3 124438-73-9 314064-67-0 RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of (heterocyclyl)alkoxy benzaldehyde oximes as antiviral agents)

IT 5198-85-6P 113079-60-0P 314064-59-0P 314064-60-3P 314064-61-4P 314064-62-5P 314064-63-6P 314064-64-7P 314064-65-8P 314064-66-9P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of (heterocyclyl)alkoxy benzaldehyde oximes as antiviral agents)

RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD RE

(1) Bayer Ag; EP 290906 A 1988 HCAPLUS

- (2) Bayer Aktiengesellschaft; US 4472416 A 1984 HCAPLUS
- (3) Kumiai Chem Ind Co Ltd; JP 8081314 A 1996
- (4) Malamas; J Med Chem 1996, V39(1), P237 HCAPLUS
- (5) Starling; Indian Journal of chemistry 1977, V15(8), P715 HCAPLUS
- (6) Strupczewski; J Med Chem 1995, V38(7), P1119 HCAPLUS
- (7) Teijin Limited; WO 9001874 1990 HCAPLUS
- (8) Teijin Ltd; JP 05320117 A 1993 HCAPLUS
- IT 314062-80-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of (heterocyclyl)alkoxy benzaldehyde oximes as antiviral agents)

RN 314062-80-1 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

Me
$$N$$
 N CH_2-CH_2-O

IT 314062-79-8P 314062-81-2P 314062-82-3P 314062-83-4P 314062-84-5P 314062-85-6P 314062-86-7P 314062-87-8P 314062-88-9P 314062-89-0P 314062-90-3P 314062-91-4P 314062-92-5P 314062-93-6P 314062-94-7P 314062-95-8P 314062-96-9P 314062-97-0P 314062-98-1P 314063-00-8P 314063-01-9P 314063-02-0P 314063-04-2P 314063-05-3P 314063-06-4P 314063-07-5P 314063-08-6P 314063-09-7P 314063-10-0P 314063-11-1P 314063-12-2P 314063-13-3P 314063-15-5P 314063-16-6P 314063-17-7P 314063-18-8P 314063-19-9P 314063-20-2P 314063-22-4P 314063-23-5P 314063-25-7P 314063-26-8P 314063-27-9P 314063-28-0P 314063-32-6P

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314063-33-7P 314063-35-9P 314063-36-0P
314063-37-1P 314063-38-2P 314063-39-3P
314063-40-6P 314063-41-7P 314063-42-8P
314063-43-9P 314063-44-0P 314063-45-1P
314063-46-2P 314063-47-3P 314063-48-4P
314063-51-9P 314063-52-0P 314063-53-1P
314063-55-3P 314063-57-5P 314063-59-7P
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314064-27-2P 314064-28-3P 314064-29-4P
314064-30-7P 314064-31-8P 314064-32-9P
314064-33-0P 314064-34-1P 314064-36-3P
314064-40-9P 314064-44-3P 314064-46-5P
314064-47-6P 314064-48-7P 314064-49-8P
314064-50-1P 314064-51-2P 314064-52-3P
314064-53-4P 314064-54-5P 314064-55-6P
314064-56-7P 314064-57-8P 314064-58-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
   (preparation of (heterocyclyl)alkoxy benzaldehyde oximes as antiviral
   agents)
314062-79-8 HCAPLUS
Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-,
O-ethyloxime (9CI) (CA INDEX NAME)
```

$$CH = N - OEt$$

$$CH_2 - CH_2 - O$$

RN

CN

RN 314062-81-2 HCAPLUS CN Ethanone, 1-[4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]phenyl]-, O-ethyloxime (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{N-OEt} \\ \parallel \\ \text{C-Me} \end{array}$$

RN 314062-82-3 HCAPLUS

CN Ethanone, 1-[4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]phenyl]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314062-83-4 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-3-methoxy-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314062-84-5 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-3,5-dimethoxy-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314062-85-6 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)

Me
$$N$$
 N CH_2-CH_2-O CH $N-OMe$

RN 314062-86-7 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Cl} & \text{N} & \text{CH} = \text{N-OMe} \\ \hline & \text{N} & \text{CH}_2 - \text{CH}_2 - \text{O} \\ \hline \end{array}$$

RN 314062-87-8 HCAPLUS

CN Ethanone, 1-[4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]phenyl], O-methyloxime (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{N-OMe} \\ \parallel \\ \text{C-Me} \end{array}$$

RN 314062-88-9 HCAPLUS

CN 1-Propanone, 1-[4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]phenyl]-, 0-methyloxime (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{N-OMe} \\ \parallel \\ \text{C-Et} \end{array}$$

RN 314062-89-0 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-propyloxime (9CI) (CA INDEX NAME)

$$CH = N - OPr - n$$
 $N = CH_2 - CH_2 - O$

RN 314062-90-3 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-(1-methylethyl)oxime (9CI) (CA INDEX NAME)

C1
$$N$$
 N CH_2-CH_2-O CH_3-O

RN 314062-91-4 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-2-propenyloxime (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{C1} & \text{N} & \text{CH} = \text{N-O-CH}_2 - \text{CH} = \text{CH}_2 \\ \hline & \text{N} & \text{N} & \text{CH}_2 - \text{CH}_2 - \text{O} \\ \hline \end{array}$$

RN 314062-92-5 HCAPLUS

CN Acetonitrile, [[[[4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]phenyl]methylene]amino]oxy]- (9CI) (CA INDEX NAME)

$$C1$$
 N
 $CH = N-O-CH_2-CN$
 $CH = N-O-CH_2-CN$

RN 314062-93-6 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-(phenylmethyl)oxime (9CI) (CA INDEX NAME)

$$CH = N - O - CH_2 - Ph$$
 $CH = N - O - CH_2 - Ph$

RN 314062-94-7 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-3,5-

dimethyl-, O-methyloxime (9CI) (CA INDEX NAME)

RN 314062-95-8 HCAPLUS

CN Ethanone, 1-[4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-3-methoxyphenyl]-, O-methyloxime (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & N-\text{OMe} \\ \parallel & \\ C-\text{Me} \\ \end{array}$$

RN 314062-96-9 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-[2-[2-(ethyldioxy)ethoxy]ethyl]oxime (9CI) (CA INDEX NAME)

C1
$$N$$
 N CH_2-CH_2-O CH_2-CH_2-O

PAGE 1-B

- CH₂- CH₂- O- OEt

RN 314062-97-0 HCAPLUS

CN Benzaldehyde, 4-[2-[1-[6-(2,2,2-trifluoroethoxy)-3-pyridazinyl]-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314062-98-1 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-methoxy-3-pyridazinyl)-4-piperidinyl]ethoxy]-,

O-ethyloxime (9CI) (CA INDEX NAME)

MeO
$$N$$
 N CH_2-CH_2-O $CH=N-OEt$

RN 314063-00-8 HCAPLUS

CN Benzaldehyde, 4-[[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]methoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314063-01-9 HCAPLUS

CN Benzaldehyde, 4-[3-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]propoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314063-02-0 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-3-methoxy-, O-methyloxime (9CI) (CA INDEX NAME)

$$CH_2-CH_2-O$$
OMe

 CH_2-CH_2-O

RN 314063-04-2 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-3-nitro-, O-ethyloxime (9CI) (CA INDEX NAME)

$$CH_2-CH_2-O$$
 NO_2
 CH_2-O
 NO_2

RN 314063-05-3 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-2-hydroxy-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314063-06-4 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-3-methyl-, O-ethyloxime (9CI) (CA INDEX NAME)

$$CH_2-CH_2-O$$
 Me
 CH_2-CH_2-O
 Me

RN 314063-07-5 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-3-methyl-, O-2-propenyloxime (9CI) (CA INDEX NAME)

RN 314063-08-6 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-3-methyl-, O-methyloxime (9CI) (CA INDEX NAME)

$$CH_2-CH_2-O$$
 Me
 CH_2-CH_2-O
 Me

RN 314063-09-7 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-3,5-dimethyl-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314063-10-0 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314063-11-1 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-2-methoxy-, O-ethyloxime (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{OMe} \\ \text{C1} & \text{N} \\ \text{N} & \text{CH}_2\text{-}\text{CH}_2\text{-}\text{O} \end{array}$$

RN 314063-12-2 HCAPLUS

CN Benzaldehyde, 3-methyl-4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{CH} & \text{N-OEt} \\ \text{N} & \text{N} \end{array}$$

RN 314063-13-3 HCAPLUS

CN Benzaldehyde, 3-methyl-4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, 0-methyloxime (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{CH} = \text{N-OMe} \\ \text{CH}_2 - \text{CH}_2 - \text{O} \\ \text{Me} \end{array}$$

RN 314063-15-5 HCAPLUS

CN Benzaldehyde, 3-methyl-4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-propyloxime (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CH & N-OPr-n \\ \hline \\ Me & N \end{array}$$

RN 314063-16-6 HCAPLUS

CN Benzaldehyde, 4-[[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]oxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314063-17-7 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-phenyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314063-18-8 HCAPLUS

CN 1-Propanone, 1-[4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]phenyl]-, O-ethyloxime, (1Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 314063-19-9 HCAPLUS

CN Benzaldehyde, 4-[2-[1-[6-(trifluoromethyl)-3-pyridazinyl]-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

$$CF_3$$

RN 314063-20-2 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-(2,2,2-trifluoroethyl)oxime (9CI) (CA INDEX NAME)

Me N
$$\sim$$
 CH $_2$ CH $_2$ CH $_2$ CH $_3$

RN 314063-22-4 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-propyloxime (9CI) (CA INDEX NAME)

Me N
$$\sim$$
 CH $_2$ CH $_2$ - O \sim CH $=$ N-OPr-n

RN 314063-23-5 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-(2-methoxyethyl)oxime (9CI) (CA INDEX NAME)

Me N
$$\sim$$
 CH $_2$ - CH $_2$ - OMe \sim N \sim CH $_2$ - CH $_2$ - OMe

RN 314063-25-7 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-2-propynyloxime (9CI) (CA INDEX NAME)

Me
$$N - CH_2 -$$

RN 314063-26-8 HCAPLUS

CN Benzaldehyde, 4-[3-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]propoxy]-, O-methyloxime (9CI) (CA INDEX NAME)

RN 314063-27-9 HCAPLUS

CN Benzaldehyde, 4-[3-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]propoxy]-, O-methyloxime (9CI) (CA INDEX NAME)

RN 314063-28-0 HCAPLUS

CN Benzaldehyde, 4-[3-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]propoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314063-32-6 HCAPLUS

CN 3-Pyridazinecarboxaldehyde, 6-[4-[2-[4-[(ethoxyimino)methyl]phenoxy]ethyl]-1-piperidinyl]- (9CI) (CA INDEX NAME)

RN 314063-33-7 HCAPLUS

CN Benzaldehyde, 4-[2-[1-[6-(hydroxymethyl)-3-pyridazinyl]-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

$$CH = N - OEt$$
 $N = CH_2 - CH_2 - O$
 $N = N - OEt$

RN 314063-35-9 HCAPLUS

CN Benzaldehyde, 3-hydroxy-4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{CH} = \text{N-OEt} \\ \text{OH} \\ \text{N} \end{array}$$

RN 314063-36-0 HCAPLUS

CN Benzaldehyde, 2,6-dimethyl-4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314063-37-1 HCAPLUS

CN Benzaldehyde, 2,6-dimethyl-4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{N} \\ \text{N} \\ \text{N} \\ \text{Me} \end{array}$$

RN 314063-38-2 HCAPLUS

CN Benzaldehyde, 2-methoxy-4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

Me
$$N$$
 N CH_2-CH_2-O CH_2-O

RN 314063-39-3 HCAPLUS

CN Benzaldehyde, 2-methyl-4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

Me
$$\sim$$
 CH $=$ N $=$ OEt

RN 314063-40-6 HCAPLUS

CN Benzaldehyde, 2-methyl-4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{N} \\ \text{N} \\ \text{N} \\ \text{N} \\ \text{CH}_2 - \text{CH}_2 - \text{O} \\ \end{array}$$

RN 314063-41-7 HCAPLUS

CN Benzaldehyde, 2,5-dimethyl-4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314063-42-8 HCAPLUS

CN Benzaldehyde, 2,5-dimethyl-4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)

Me
$$\sim$$
 CH $=$ N $=$ OMe \sim Me \sim Me \sim Me \sim Me \sim Me

RN 314063-43-9 HCAPLUS

CN Benzaldehyde, 2,3-dimethyl-4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

Me Me
$$CH = N - OEt$$

$$CH_2 - CH_2 - O$$

RN 314063-44-0 HCAPLUS

CN Benzaldehyde, 2,3-dimethyl-4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)

RN 314063-45-1 HCAPLUS

CN 3-Pyridazinecarboxaldehyde, 6-[4-[2-[4-[(ethoxyimino)methyl]phenoxy]ethyl]-1-piperidinyl]-, O-methyloxime (9CI) (CA INDEX NAME)

MeO-N=CH N
$$\sim$$
 CH2-CH2-O

RN 314063-46-2 HCAPLUS

CN Benzaldehyde, 3-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)

RN 314063-47-3 HCAPLUS

CN Benzaldehyde, 3-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-4-methoxy-, O-methyloxime (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{MeO-N-CH} \\ & \text{CH}_2\text{-CH}_2\text{-O} \\ & \text{OMe} \end{array}$$

RN 314063-48-4 HCAPLUS

CN Benzaldehyde, 3-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-5-hydroxy-, O-methyloxime (9CI) (CA INDEX NAME)

MeO-N-CH
$$\sim$$
 CH \sim CH

RN 314063-51-9 HCAPLUS

CN Benzaldehyde, 3-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314063-52-0 HCAPLUS

CN Benzaldehyde, 3-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

Me
$$N$$
 N CH_2-CH_2-O CH N OEt

RN 314063-53-1 HCAPLUS

CN Benzaldehyde, 3-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-2-propenyloxime (9CI) (CA INDEX NAME)

RN 314063-55-3 HCAPLUS

CN Benzaldehyde, 3-[[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]methoxy]-, O-methyloxime (9CI) (CA INDEX NAME)

$$C1$$
 N
 $CH=N-OMe$

RN 314063-57-5 HCAPLUS

CN Benzaldehyde, 3-[[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]methoxy]-, 0-2-propenyloxime (9CI) (CA INDEX NAME)

$$C1$$
 N
 $CH=N-O-CH_2-CH=CH_2$

RN 314063-59-7 HCAPLUS

CN Benzaldehyde, 3-[3-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]propoxy]-,
O-ethyloxime (9CI) (CA INDEX NAME)

RN 314063-60-0 HCAPLUS

CN Benzaldehyde, 3-[3-[1-(6-methoxy-3-pyridazinyl)-4-piperidinyl]propoxy]-, O-methyloxime (9CI) (CA INDEX NAME)

MeO-N=CH O- (CH₂)
$$_3$$
 OMe

314063-61-1 HCAPLUS RN

Benzaldehyde, 3-[3-[1-(6-methoxy-3-pyridazinyl)-4-piperidinyl]propoxy]-, CNO-ethyloxime (9CI) (CA INDEX NAME)

Eto-N=CH O- (CH₂)
$$_3$$
 OMe

314063-64-4 HCAPLUS RN

Benzaldehyde, 3-[3-[1-(3-pyridazinyl)-4-piperidinyl]propoxy]-, CNO-ethyloxime (9CI) (CA INDEX NAME)

314063-66-6 HCAPLUS RN

1H-Inden-1-one, 2,3-dihydro-4-[2-[1-(6-methyl-3-pyridazinyl)-4-CNpiperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314063-67-7 HCAPLUS

CN Benzaldehyde, 3,5-dimethyl-4-[3-(3-methyl-5-isoxazolyl)propoxy]-, O-methyloxime (9CI) (CA INDEX NAME)

prlr

RN 314063-68-8 HCAPLUS

CN Benzaldehyde, 3,5-dimethyl-4-[3-(3-methyl-5-isoxazolyl)propoxy]-, O-2-propenyloxime (9CI) (CA INDEX NAME)

 H_2C —CH— CH_2 —O—N—CH

RN 314063-69-9 HCAPLUS

CN Benzaldehyde, 3,5-dimethyl-4-[3-(3-methyl-5-isoxazolyl)propoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314063-70-2 HCAPLUS
CN Benzaldehyde, 3,5-dimethyl-4-[3-(3-methyl-5-isoxazolyl)propoxy]-,
O-(phenylmethyl)oxime (9CI) (CA INDEX NAME)

Me
$$(CH_2)_3$$
 O
 Me
 $Ph-CH_2-O-N$
 CH

RN 314063-71-3 HCAPLUS
CN Benzaldehyde, 4-[3-(3-methyl-5-isoxazolyl)propoxy]-, 0-ethyloxime (9CI)
(CA INDEX NAME)

RN 314063-72-4 HCAPLUS

CN Ethanone, 1-[3,5-dimethyl-4-[3-(3-methyl-5-isoxazolyl)propoxy]phenyl]-, O-methyloxime (9CI) (CA INDEX NAME)

RN 314063-73-5 HCAPLUS
CN Benzaldehyde, 3,5-dimethyl-4-[3-(3-methyl-5-isoxazolyl)propoxy]-,
O-propyloxime (9CI) (CA INDEX NAME)

RN 314063-74-6 HCAPLUS
CN Acetonitrile, [[[[3,5-dimethyl-4-[3-(3-methyl-5-isoxazolyl)propoxy]phenyl]methylene]amino]oxy]- (9CI) (CA INDEX NAME)

RN 314063-75-7 HCAPLUS

CN Benzaldehyde, 3,5-dimethyl-4-[3-(3-methyl-5-isoxazolyl)propoxy]-, O-2-propynyloxime (9CI) (CA INDEX NAME)

 $HC = C - CH_2 - O - N = CH$

RN 314063-76-8 HCAPLUS
CN Benzaldehyde, 3,5-dimethyl-4-[[6-(3-methyl-5-isoxazolyl)hexyl]oxy]-,
O-ethyloxime (9CI) (CA INDEX NAME)

Me
$$N$$
 O $(CH_2)_6$ O Me Me Me Me

RN 314063-77-9 HCAPLUS

CN Benzaldehyde, 3,5-dimethyl-4-[[7-(3-methyl-5-isoxazolyl)heptyl]oxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314063-78-0 HCAPLUS

CN Benzaldehyde, 3,5-dimethyl-4-[[5-(3-methyl-5-isoxazolyl)pentyl]oxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314063-79-1 HCAPLUS

CN Benzaldehyde, 3,5-dimethyl-4-[4-(3-methyl-5-isoxazolyl)butoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314063-80-4 HCAPLUS

CN Benzaldehyde, 3,5-dimethyl-4-[3-(3-methyl-5-isoxazolyl)propoxy]-, O-(2,2,2-trifluoroethyl)oxime (9CI) (CA INDEX NAME)

 $F_3C-CH_2-O-N=-CH$

RN 314063-81-5 HCAPLUS

CN Benzaldehyde, 3,5-dimethyl-4-[3-(3-methyl-5-isoxazolyl)propoxy]-, O-(2-ethoxyethyl)oxime (9CI) (CA INDEX NAME)

RN 314063-82-6 HCAPLUS

CN Benzaldehyde, 3,5-dimethyl-4-[3-(3-methyl-5-isoxazolyl)propoxy]-, O-(2-oxopropyl)oxime (9CI) (CA INDEX NAME)

RN 314063-83-7 HCAPLUS
CN Benzaldehyde, 3,5-dimethyl-4-[3-(3-phenyl-5-isoxazolyl)propoxy]-,
O-ethyloxime (9CI) (CA INDEX NAME)

Et
$$N$$
 O $(CH_2)_3$ O Me Me $EtO-N$ CH

RN 314063-85-9 HCAPLUS

CN Benzaldehyde, 3,5-dimethyl-4-[3-(3-propyl-5-isoxazolyl)propoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314063-86-0 HCAPLUS

CN Benzaldehyde, 4-[2-(3-ethyl-5-isoxazolyl)ethoxy]-3,5-dimethyl-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314063-87-1 HCAPLUS

CN Benzaldehyde, 3,5-dimethyl-4-[3-(3-methyl-5-isoxazolyl)propoxy]-, O-(2-fluoroethyl)oxime (9CI) (CA INDEX NAME)

 $FCH_2 - CH_2 - O - N = CH$

RN 314063-89-3 HCAPLUS

CN Benzaldehyde, 4-[4-(3-ethyl-5-isoxazolyl)butoxy]-3,5-dimethyl-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314063-90-6 HCAPLUS

CN Benzaldehyde, 3,5-dimethyl-4-[4-(3-propyl-5-isoxazolyl)butoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314063-91-7 HCAPLUS

CN Benzaldehyde, 4-[2-[4-(6-chloro-3-pyridazinyl)-1-piperazinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314063-95-1 HCAPLUS

CN Benzaldehyde, 4-[2-[4-(6-methyl-3-pyridazinyl)-1-piperazinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)

Me N N
$$\sim$$
 CH $_2$ - CH $_2$ - O \sim CH \sim N \sim OMe

RN 314063-96-2 HCAPLUS

CN Benzaldehyde, 4-[2-[4-(6-methyl-3-pyridazinyl)-1-piperazinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

Me N N
$$\sim$$
 CH $_2$ - CH $_2$ - O

RN 314063-98-4 HCAPLUS

CN Benzaldehyde, 3-[2-[4-(6-methyl-3-pyridazinyl)-1-piperazinyl]ethoxyl-, O-methyloxime (9CI) (CA INDEX NAME)

RN 314063-99-5 HCAPLUS

CN Benzaldehyde, 3-[2-[4-(6-methyl-3-pyridazinyl)-1-piperazinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314064-01-2 HCAPLUS

CN Benzaldehyde, 4-[2-[4-(6-chloro-3-pyridazinyl)-1-piperazinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)

C1
$$N$$
 N N CH_2 CH_2 O

RN 314064-03-4 HCAPLUS

CN Benzaldehyde, 3-[2-[4-(6-chloro-3-pyridazinyl)-1-piperazinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)

RN 314064-04-5 HCAPLUS

CN Benzaldehyde, 3-[2-[4-(6-chloro-3-pyridazinyl)-1-piperazinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314064-05-6 HCAPLUS

CN Benzaldehyde, 3-[2-[4-(6-chloro-3-pyridazinyl)-1-piperazinyl]ethoxy]-, O-2-propenyloxime (9CI) (CA INDEX NAME)

RN 314064-06-7 HCAPLUS

CN Benzaldehyde, 4-[2-[4-(6-methyl-3-pyridazinyl)-1-piperazinyl]ethoxy]-, O-propyloxime (9CI) (CA INDEX NAME)

Me N N N
$$\sim$$
 CH $_2$ - CH $_2$ - O

RN 314064-07-8 HCAPLUS

CN Benzaldehyde, 3-[2-[4-(6-methyl-3-pyridazinyl)-1-piperazinyl]ethoxy]-,
O-propyloxime (9CI) (CA INDEX NAME)

Me N N
$$\sim$$
 CH2 \sim CH2 \sim CH N \sim OPr \sim N

RN 314064-08-9 HCAPLUS

CN Benzaldehyde, 3-[2-[4-(6-chloro-3-pyridazinyl)-1-piperazinyl]ethoxy]-, O-propyloxime (9CI) (CA INDEX NAME)

RN 314064-09-0 HCAPLUS

CN Benzaldehyde, 4-[[1-(6-chloro-3-pyridazinyl)-3-piperidinyl]methoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314064-13-6 HCAPLUS

CN Benzaldehyde, 4-[3-[1-(6-chloro-3-pyridaziny1)-3-piperidinyl]propoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314064-14-7 HCAPLUS

CN Benzaldehyde, 3-[3-[1-[6-(trifluoromethyl)-3-pyridazinyl]-3-piperidinyl]propoxy]-, O-methyloxime (9CI) (CA INDEX NAME)

MeO-N=CH O- (CH₂)₃ N N N
$$_{\text{CF}}$$

RN 314064-15-8 HCAPLUS

CN Benzaldehyde, 3-[3-[1-[6-(trifluoromethyl)-3-pyridazinyl]-3-piperidinyl]propoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314064-16-9 HCAPLUS

CN Benzaldehyde, 3-[3-[1-(6-methyl-3-pyridazinyl)-3-piperidinyl]propoxy]-, O-methyloxime (9CI) (CA INDEX NAME)

RN 314064-17-0 HCAPLUS

CN Benzaldehyde, 3-[3-[1-(6-methyl-3-pyridazinyl)-3-piperidinyl]propoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314064-18-1 HCAPLUS

CN Benzaldehyde, 3-[[1-(6-chloro-3-pyridazinyl)-3-piperidinyl]methoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314064-19-2 HCAPLUS
CN Benzaldehyde, 4-[[1-[6-(trifluoromethyl)-3-pyridazinyl]-3-piperidinyl]methoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314064-20-5 HCAPLUS
CN Benzaldehyde, 3-[[1-[6-(trifluoromethyl)-3-pyridazinyl]-3-piperidinyl]methoxy]-, O-methyloxime (9CI) (CA INDEX NAME)

$$_{\text{CH}}$$
 $_{\text{N}}$ $_{\text{CH}}$ $_{\text{CH}}$ $_{\text{N}}$ $_{\text{OMe}}$

RN 314064-21-6 HCAPLUS
CN Benzaldehyde, 3-[[1-[6-(trifluoromethyl)-3-pyridazinyl]-3-piperidinyl]methoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314064-22-7 HCAPLUS
CN Benzaldehyde, 4-[2-[1-[5-(trifluoromethyl)-2-pyridinyl]-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314064-24-9 HCAPLUS

CN Benzaldehyde, 4-[2-[1-[5-(trifluoromethyl)-1,3,4-thiadiazol-2-yl]-4-piperidinyl]ethoxy]-, 0-methyloxime (9CI) (CA INDEX NAME)

$$CH = N - OMe$$

RN 314064-25-0 HCAPLUS

CN Benzaldehyde, 4-[2-[1-[5-(trifluoromethyl)-1,3,4-thiadiazol-2-yl]-4-piperidinyl]ethoxy]-, 0-ethyloxime (9CI) (CA INDEX NAME)

$$CH_2 - CH_2 - O$$
 $CH = N - OEt$

RN 314064-26-1 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(5-methyl-1,3,4-thiadiazol-2-yl)-4-piperidinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)

RN 314064-27-2 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(5-methyl-1,3,4-thiadiazol-2-yl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

$$N$$
 S
 $CH = N - OEt$
 Me

RN 314064-28-3 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(5-chloropyrazinyl)-4-piperidinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{C1} & \text{CH} & \text{N-OMe} \\ \hline \\ \text{N} & \text{N} & \text{CH}_2\text{-CH}_2\text{-O} \end{array}$$

RN 314064-29-4 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(5-chloropyrazinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314064-30-7 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-methyl-2-pyridinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & &$$

RN 314064-31-8 HCAPLUS

CN 4-Thiazolecarboxylic acid, 2-[4-[2-[4-[(methoxyimino)methyl]phenoxy]ethyl]-1-piperidinyl]-, ethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & \\ \parallel & & \\ EtO-C & N & \\ \hline & N & \\ \hline & CH=N-OMe \end{array}$$

RN 314064-32-9 HCAPLUS

CN 4-Thiazolecarboxylic acid, 2-[4-[2-[4-[(ethoxyimino)methyl]phenoxy]ethyl]-1-piperidinyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 314064-33-0 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-chloropyrazinyl)-4-piperidinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)

RN 314064-34-1 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(2-benzoxazolyl)-4-piperidinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CH_2-CH_2-O \\ \hline \\ CH \end{array}$$

RN 314064-36-3 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(4,6-dimethoxy-1,3,5-triazin-2-yl)-4-piperidinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{OMe} \\ \text{N} \\ \text{N} \\ \text{O-CH}_2\text{-CH}_2 \\ \end{array}$$

RN 314064-40-9 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(5-ethyl-2-pyrimidinyl)-4-piperidinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Et} & \text{N-OMe} \\ \hline \\ N & \text{N-N-OMe} \\ \end{array}$$

RN 314064-44-3 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(2-benzothiazolyl)-4-piperidinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{CH}_2-\text{CH}_2-\text{O} \\ \hline \\ \text{CH} \end{array}$$

RN 314064-46-5 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(2-benzothiazolyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314064-47-6 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-chloro-2-quinoxalinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314064-48-7 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-chloro-5-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314064-49-8 HCAPLUS

CN Benzaldehyde, 4-[[5-[(6-chloro-3-pyridazinyl)amino]pentyl]oxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

RN 314064-50-1 HCAPLUS

CN Benzaldehyde, 4-[[5-[(6-chloro-3-pyridazinyl)methylamino]pentyl]oxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} & \\ \hline & \text{O-} (\text{CH}_2)_5 - \text{N} \\ \hline \end{array}$$

RN 314064-51-2 HCAPLUS

CN Benzaldehyde, 4-[[6-[(6-chloro-3-pyridazinyl)amino]hexyl]oxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

RN 314064-52-3 HCAPLUS

CN Benzaldehyde, 4-[4-[(6-chloro-3-pyridazinyl)amino]butoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314064-53-4 HCAPLUS

CN Benzaldehyde, 4-[[6-[(6-chloro-3-pyridazinyl)methylamino]hexyl]oxy]-, O-methyloxime (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{Me} \\ \hline \\ \text{O-} & \text{(CH_2)} & \text{6} \\ \hline \end{array}$$

RN 314064-54-5 HCAPLUS

CN Benzaldehyde, 4-[4-[(6-chloro-3-pyridazinyl)methylamino]butoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} \\ & & \\ \hline & \text{O-} (\text{CH}_2)_4 - \text{N} \\ & & \\ \hline & \text{EtO-} \text{N} \\ \end{array}$$

RN 314064-55-6 HCAPLUS

CN Benzaldehyde, 4-[[5-[(6-chloro-3-pyridazinyl)oxy]pentyl]oxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314064-56-7 HCAPLUS

CN Benzaldehyde, 4-[(6-chloro-2-quinoxalinyl)oxy]-, O-ethyloxime (9CI) (CAINDEX NAME)

RN 314064-57-8 HCAPLUS

CN 4-Thiazolecarboxaldehyde, 2-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, 0-ethyloxime (9CI) (CA INDEX NAME)

Eto-N=CH
$$N$$
 O-CH₂-CH₂ N N N N

RN 314064-58-9 HCAPLUS

CN 4-Thiazolecarboxaldehyde, 2-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, 0-methyloxime (9CI) (CA INDEX NAME)

$$\mathsf{MeO-N} = \mathsf{CH} \qquad \mathsf{N} \qquad \mathsf{$$

TT 314062-99-2 314063-03-1 314063-14-4 314063-21-3 314063-24-6 314063-29-1 314063-30-4 314063-31-5 314063-34-8 314063-49-5 314063-50-8 314063-54-2 314063-56-4 314063-58-6 314063-62-2 314063-63-3 314063-65-5 314063-88-2 314063-92-8 314063-93-9 314063-94-0 314063-97-3 314064-00-1 314064-02-3 314064-10-3 314064-11-4 314064-12-5 314064-35-2 314064-38-5 314064-42-1 314255-60-2

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(preparation of (heterocyclyl)alkoxy benzaldehyde oximes as antiviral agents)

RN 314062-99-2 HCAPLUS

CN Benzaldehyde, 4-[[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]methoxy]-, O-2-propenyloxime (9CI) (CA INDEX NAME)

$$CH = N - O - CH_2 - CH = CH_2$$

RN 314063-03-1 HCAPLUS

CN 1-Propanone, 1-[4-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]phenyl]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314063-14-4 HCAPLUS

CN Benzaldehyde, 3-methyl-4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-2-propenyloxime (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{CH} = \text{N-O-CH}_2 - \text{CH} = \text{CH}_2 \\ \text{Me} \end{array}$$

RN 314063-21-3 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-methoxy-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-2-propenyloxime (9CI) (CA INDEX NAME)

MeO N N
$$CH = N - O - CH_2 - CH = CH_2$$

RN 314063-24-6 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-2-propenyloxime (9CI) (CA INDEX NAME)

RN 314063-29-1 HCAPLUS

CN Benzaldehyde, 4-[3-[1-[6-(trifluoromethyl)-3-pyridazinyl]-4-piperidinyl]propoxy]-, O-methyloxime (9CI) (CA INDEX NAME)

RN 314063-30-4 HCAPLUS

CN Benzaldehyde, 4-[3-[1-(3-pyridazinyl)-4-piperidinyl]propoxy]-, O-methyloxime (9CI) (CA INDEX NAME)

RN 314063-31-5 HCAPLUS

CN Benzaldehyde, 4-[3-[1-(3-pyridazinyl)-4-piperidinyl]propoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314063-34-8 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-(2-fluoroethyl)oxime (9CI) (CA INDEX NAME)

Me
$$N \longrightarrow CH_2 - CH_2 - O$$
 $CH \longrightarrow N \longrightarrow CH_2 - CH_2 F$

RN 314063-49-5 HCAPLUS

CN Benzaldehyde, 3-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-5-

hydroxy-, O-ethyloxime (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{EtO-N-CH} \\ & \text{CH}_2\text{-CH}_2\text{-O} \\ & \text{OH} \end{array}$$

RN 314063-50-8 HCAPLUS

CN Benzaldehyde, 3-[2-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]ethoxy]-5-hydroxy-, O-2-propenyloxime (9CI) (CA INDEX NAME)

$$H_2C = CH - CH_2 - O - N = CH$$
 $CH_2 - CH_2 - O - N = CH$
 $CH_2 - CH_2 - O - N = CH$
 $CH_2 - CH_2 - O - N = CH$

RN 314063-54-2 HCAPLUS

CN Benzaldehyde, 3-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)

RN 314063-56-4 HCAPLUS

CN Benzaldehyde, 3-[[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]methoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314063-58-6 HCAPLUS

CN Benzaldehyde, 3-[3-[1-(6-chloro-3-pyridazinyl)-4-piperidinyl]propoxy]-,
O-methyloxime (9CI) (CA INDEX NAME)

$$H_2C = CH - CH_2 - O - N = CH$$
O— $(CH_2)_3$
OMe

RN 314063-63-3 HCAPLUS CN Benzaldehyde, 3-[3-[1-(3-pyridazinyl)-4-piperidinyl]propoxy]-, O-methyloxime (9CI) (CA INDEX NAME)

RN 314063-65-5 HCAPLUS CN Benzaldehyde, 3-[3-[1-(3-pyridazinyl)-4-piperidinyl]propoxy]-, O-2-propenyloxime (9CI) (CA INDEX NAME)

$$\sim$$
 CH \sim N \sim CH \sim

RN 314063-88-2 HCAPLUS
CN Benzaldehyde, 4-[3-(3-cyclopropyl-5-isoxazolyl)propoxy]-3,5-dimethyl-,
O-ethyloxime (9CI) (CA INDEX NAME)

RN 314063-92-8 HCAPLUS

CN Benzaldehyde, 4-[2-[4-(3-pyridazinyl)-1-piperazinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314063-93-9 HCAPLUS

CN Benzaldehyde, 3-[2-[4-(3-pyridazinyl)-1-piperazinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314063-94-0 HCAPLUS

CN Benzaldehyde, 4-[2-[4-(3-pyridazinyl)-1-piperazinyl]ethoxy]-, O-2-propenyloxime (9CI) (CA INDEX NAME)

RN 314063-97-3 HCAPLUS

CN Benzaldehyde, 4-[2-[4-(6-methyl-3-pyridazinyl)-1-piperazinyl]ethoxy]-, O-2-propenyloxime (9CI) (CA INDEX NAME)

Me N N
$$\sim$$
 CH2 \sim CH

RN 314064-00-1 HCAPLUS

CN Benzaldehyde, 3-[2-[4-(6-methyl-3-pyridazinyl)-1-piperazinyl]ethoxy]-, O-2-propenyloxime (9CI) (CA INDEX NAME)

Me N N
$$CH_2-CH_2-O$$
 $CH=N-O-CH_2-CH=CH_2$

RN 314064-02-3 HCAPLUS

CN Benzaldehyde, 4-[2-[4-(6-chloro-3-pyridazinyl)-1-piperazinyl]ethoxy]-, O-2-propenyloxime (9CI) (CA INDEX NAME)

RN 314064-10-3 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-3-piperidinyl]ethoxy]-, O-methyloxime (9CI) (CA INDEX NAME)

$$C1$$
 N
 N
 $CH=N-OMe$

RN 314064-11-4 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-3-piperidinyl]ethoxy]-, O-2-propenyloxime (9CI) (CA INDEX NAME)

$$C1$$
 N
 $CH = N - O - CH_2 - CH = CH_2$
 $CH_2 - CH_2 - CH_2 - O$

RN 314064-12-5 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(6-chloro-3-pyridazinyl)-3-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

$$C1$$
 N
 $CH = N - OEt$
 $CH_2 - CH_2 - O$

RN 314064-35-2 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(2-benzoxazolyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314064-38-5 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(4,6-dimethoxy-1,3,5-triazin-2-yl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314064-42-1 HCAPLUS

CN Benzaldehyde, 4-[2-[1-(5-ethyl-2-pyrimidinyl)-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

RN 314255-60-2 HCAPLUS

CN Benzaldehyde, 4-[2-[1-[6-methyloxido-3-pyridazinyl]-4-piperidinyl]ethoxy]-, O-ethyloxime (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

=> => d all hitstr tot 187

L87 ANSWER 1 OF HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2004: 220079 HCAPLUS

DN 140:253575

ED Entered STN: 19 Mar 2004

TI Preparation of heteroaryl-substituted pyrrole derivatives that inhibit production of $\text{TNF}\alpha$

IN Kimura, Tomio; Aoki, Kazumasa; Nakao, Akira; Ushiyama, Shigeru; Shimozato, Takaichi; Ohkawa, Nobuyuki; Nagasaki, Takayoshi; Yamazaki, Takanori

PA Sankyo Company, Limited, Japan

SO U.S. Pat. Appl. Publ., 244 pp., Cont.-in-part of U.S. Ser. No. 317,748, abandoned.

CODEN: USXXCO

DT Patent

LA English

IC ICM C07D417-14

ICS C07D413-14; C07D043-14

NCL 544060000; 544141000; 544295000; 544333000; 546193000; 546269700;

546271400; 546272700; 546276400

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1, 63

B1

B2

FAN.CNT 3							
	PAT	TENT NO.	KIND	DATE		APPLICATION NO.	DATE
		-					
PI /	US.	2004054173	A1	20040318)	US 2003-354648	20030130 <
`	RU	2198170	C2	20030210		RU 2000-119431	20000720 <
	ZA	2000003705	Α	20010205		ZA 2000-3705	20000721 <
	JP	2002284783	A2	20021003		JP 2002-12247	20020122
PRAI	JP	1999-205491	Α	19990721	<		
	JP	1999-369678	Α	19991227	<		
	US	2000-619898	B3	20000719			
	JP	2001-13817	A	20010122			
	US	2001-275005P	P	20010312			
	US	2002-54630	B2	20020122			

20020314

20021212

II

US 2002-99176

GI

US 2002-317748

Title compds. I [A = pyrrole; R1 = (un) substituted Ph, naphthyl, etc.; R2 = pyridinyl, pyrimidinyl, etc.; R3 = heterocyclyl] are prepared For instance, α-(p-toluenesulfonyloxy)-4-fluorobenzylisonitrile is reacted with 3-(4-pyridyl)acrylate (THF, n-BuLi, LiBr, -45°) to give 4-(ethoxycarbonyl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole. This Et ester is reduced (THF/PhMe, DIBAL), oxidized to the 4-formyl derivative (DMSO, MnO2, 50°), condensed with diethylphosphonoacetonitrile (THF, NaH). This adduct was reduced (THF/MeOH, H2-Pd/C) and reduced (THF, LAH) to give II. Compds. of the

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invention inhibit production of TNF\alpha and IL-1\beta. I are useful for
     the treatment of inflammation.
     heteroaryl pyrrole pyridine pyrimidine TNF interleukin inhbitor prepn
ST
     Intestine, disease
TT
        (Crohn's; preparation of heteroaryl-substituted pyrrole derivs. that inhibit
        production of TNF\alpha)
TT
        (absorption, inhibition of; preparation of heteroaryl-substituted pyrrole
        derivs. that inhibit production of TNF\alpha)
     Heart, disease
TT
        (ischemia; preparation of heteroaryl-substituted pyrrole derivs. that
        inhibit production of TNF\alpha)
IT
     Kidney, disease
        (nephritis; preparation of heteroaryl-substituted pyrrole derivs. that
        inhibit production of TNF\alpha)
     Allergy inhibitors
TT
     Alzheimer's disease
     Analgesics
     Anti-Alzheimer's agents
     Anti-inflammatory agents
     Antiarteriosclerotics
     Antiarthritics
     Antidiabetic agents
     Antirheumatic agents
       Antiviral agents
     Arteriosclerosis
     Diabetes mellitus
     Fever and Hyperthermia
     Hepatitis
     Human
     Lupus erythematosus
     Osteoarthritis
     Osteoporosis
     Pain
     Psoriasis
     Rheumatoid arthritis
     Septicemia
         (preparation of heteroaryl-substituted pyrrole derivs. that inhibit
production
        of TNF\alpha)
TT
     Cytokines
     Interleukin 1\beta
     Tumor necrosis factors
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
         (preparation of heteroaryl-substituted pyrrole derivs. that inhibit
production
        of TNF\alpha)
     Intestine, disease
         (ulcerative colitis; preparation of heteroaryl-substituted pyrrole derivs.
        that inhibit production of TNF\alpha)
                     321344-58-5P
IT
     321344-57-4P
     RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN
      (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study);
     PREP (Preparation); USES (Uses)
         (preparation of heteroaryl-substituted pyrrole derivs. that inhibit
production
        of TNF\alpha)
     321343-74-2P, 4-(3-Aminopropyl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-
                321343-78-6P, 4-Aminomethyl-2-(4-fluorophenyl)-3-(pyridin-4-yl)-
      TH-pyrrole Dihydrochloride 321343-82-2P, 4-(1-Acetyl-1,2,3,6-
      tetrahydropyridin-4-yl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole
      321343-83-3P, 2-(4-Fluorophenyl)-3-(pyridin-4-yl)-4-(1,2,3,6-
      tetrahydropyridin-4-yl)-1H-pyrrole dihydrochloride
                                                             321343-86-6P,
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1-(1-Benzylpiperidin-4-yl)-3-(4-fluorophenyl)-2-(pyridin-4-yl)-1H-pyrrole
     321343-87-7P, 3-(4-Fluorophenyl)-1-(piperidin-4-yl)-2-(pyridin-4-yl)-1H-
                             321344-06-3P, 2-(4-Fluorophenyl)-4-(1-methyl-
               321343-98-0P
     1,2,3,6-tetrahydropyridin-4-yl)-3-(pyridin-4-yl)-1H-pyrrole
                                                                   321344-09-6P
     321344-17-6P, 2-(4-Fluorophenyl)-4-(8-methyl-8-azabicyclo[3.2.1]oct-2-en-3-
     yl)-3-(pyridin-4-yl)-1H-pyrrole 321344-19-8P, 4-(8-Azabicyclo[3.2.1]oct-
     2-en-3-yl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole
                                                                 321344-21-2P,
     2-(4-Fluorophenyl)-3-(pyridin-4-yl)-4-(1,2,3,6-tetrahydro-2,2,6,6-
     tetramethylpyridin-4-yl)-1H-pyrrole 321344-24-5P, 2-(4-Fluorophenyl)-4-
     (6-methyl-1,2,3,6-tetrahydropyridin-4-yl)-3-(pyridin-4-yl)-1H-pyrrole
                   321344-28-9P, 2-(4-Fluorophenyl)-4-(1-isopropyl-1,2,3,6-
     321344-26-7P
     tetrahydropyridin-4-yl)-3-(pyridin-4-yl)-1H-pyrrole
                                                          321344-33-6P,
     2-(4-Fluorophenyl)-4-(1,2,3,5,8,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-
                      321344-34-7P, 2-(4-Fluorophenyl)-4-(1,2,3,5,6,8a-
     yl)-1H-pyrrole
     hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole
                                                           321344-37-0P,
     2-(4-Fluorophenyl)-4-(1,2,2,6,6-pentamethyl-1,2,3,6-tetrahydropyridin-4-
     yl)-3-(pyridin-4-yl)-1H-pyrrole
     RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
     preparation); THU (Therapeutic use); BIOL (Biological study); PREP
     (Preparation); RACT (Reactant or reagent); USES (Uses)
        (preparation of heteroaryl-substituted pyrrole derivs. that inhibit
production
     321343-75-3P, 2-(4-Fluorophenyl)-3-(pyridin-4-yl)-4-(3-
                                              321343-76-4P,
     trifluoroacetylaminopropyl)-1H-pyrrole
     4-(3-Acetylaminopropyl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole
     321343-77-5P, 2-(4-Fluorophenyl)-4-(3-methylaminopropyl)-3-(pyridin-4-yl)-
                  321343-79-7P, 2-(4-Fluorophenyl)-3-(pyridin-4-yl)-4-(2,4,6-
     1H-pyrrole
     trifluorobenzoylaminomethyl)-1H-pyrrole
                                              321343-80-0P,
     2-(4-Fluorophenyl)-3-(pyridin-4-yl)-4-(2,3,5,6-tetrafluoropyridin-4-yl)-1H-
               321343-81-1P, [5-(4-Fluorophenyl)-4-(pyridin-4-yl)-1H-pyrrol-3-
     yl] (pyridin-4-yl) methanol
                                 321343-84-4P, 2-(4-Fluorophenyl)-4-(piperidin-
                                        321343-88-8P, 3-(4-Fluorophenyl)-1-(1-
     4-yl)-3-(pyridin-4-yl)-1H-pyrrole
     methylpiperidin-4-yl)-2-(pyridin-4-yl)-1H-pyrrole
                                                         321343-89-9P,
     1-(1-Acetylpiperidin-4-yl)-3-(4-fluorophenyl)-2-(pyridin-4-yl)-1H-pyrrole
     321343-90-2P, 3-(4-Fluorophenyl)-1-[1-(2-nitroethyl)piperidin-4-yl]-2-
                                 321343-92-4P, 3-(4-Fluorophenyl)-2-(pyridin-4-
     (pyridin-4-yl)-1H-pyrrole
                                          321343-93-5P, 3-(4-Fluorophenyl)-1-
     yl) -1- (pyrrolidin-3-yl) -1H-pyrrole
     (piperidin-3-yl)-2-(pyridin-4-yl)-1H-pyrrole 321343-94-6P,
     3-(4-Fluorophenyl)-1-(piperidin-4-yl)methyl-2-(pyridin-4-yl)-1H-pyrrole
     321343-95-7P, 1-(Azetidin-3-yl)-3-(4-fluorophenyl)-2-(pyridin-4-yl)-1H-
                              321343-96-8P, 1-(3-Aminopropyl)-3-(4-
     pyrrole dihydrochloride
     fluorophenyl) -2-(pyridin-4-yl)-1H-pyrrole
                                                321343-97-9P,
     2-(4-Fluorophenyl)-3-(pyridin-4-yl)-4-[3-(thiomorpholinyl)propyl]-1H-
               321343-99-1P, 2-(4-Fluorophenyl)-4-[3-(piperazin-1-yl)propyl]-3-
                                321344-00-7P, 4-(3-Dimethylaminopropyl)-2-(4-
     (pyridin-4-yl)-1H-pyrrole
     fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole 321344-01-8P,
     2-(4-Fluorophenyl)-4-[3-(morpholinyl)propyl]-3-(pyridin-4-yl)-1H-pyrrole
     321344-02-9P, 2-(4-Fluorophenyl)-4-[3-(piperidin-1-yl)propyl]-3-(pyridin-4-
                      321344-03-0P, 2-(4-Fluorophenyl)-4-[3-(1-methylpiperazin-
     yl)-1H-pyrrole
     4-yl)propyl]-3-(pyridin-4-yl)-1H-pyrrole
                                                321344-04-1P,
     1-(3-Dimethylaminopropyl)-3-(4-fluorophenyl)-2-(pyridin-4-yl)-1H-pyrrole
     321344-05-2P, 2-(4-Fluorophenyl)-3,4-bis(pyridin-4-yl)-1H-pyrrole
     321344-07-4P, 2-(4-Fluorophenyl)-4-(1-methylpiperidin-4-yl)-3-(pyridin-4-
                     321344-08-5P, 3-(4-Fluorophenyl)-2-(pyridin-4-yl)-1-
     yl)-1H-pyrrole
     (2,2,6,6-tetramethylpiperidin-4-yl)-1H-pyrrole
                                                      321344-10-9P,
     2-(4-Fluorophenyl)-3-(pyridin-4-yl)-4-(quinuclidin-3-yl)-1H-pyrrole
     321344-11-0P, 2-(4-Fluorophenyl)-4-(4-hydroxypiperidin-4-yl)-3-(pyridin-4-
                      321344-12-1P, 2-(4-Fluorophenyl)-4-(3-
     yl)-1H-pyrrole
     ((methanesulfonyl)amino)propyl)-3-(pyridin-4-yl)-1H-pyrrole
     321344-13-2P, 3-(4-Fluorophenyl)-2-(pyridin-4-yl)-1-(quinuclidin-3-yl)-1H-
               321344-14-3P, 3-(4-Fluorophenyl)-1-(piperidin-3-yl)methyl-2-
     pyrrole
     (pyridin-4-yl)-1H-pyrrole 321344-15-4P, cis-1-(4-Aminocyclohexyl)-3-(4-
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IT

fluorophenyl) -2-(pyridin-4-yl)-1H-pyrrole 321344-16-5P, 3-(4-Fluorophenyl)-2-(2-methylaminopyrimidin-4-yl)-1-(piperidin-4-yl)-1H-321344-18-7P, 2-(4-Fluorophenyl)-4-(8-methyl-8azabicyclo[3.2.1]octan-3-yl)-3-(pyridin-4-yl)-1H-pyrrole 321344-20-1P, 4-(8-Azabicyclo[3.2.1]octan-3-yl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-321344-22-3P, 2-(4-Fluorophenyl)-3-(Pyridin-4-yl)-4-(2,2,6,6tetramethylpiperidin-4-yl)-1H-pyrrole 321344-23-4P, 2-(4-Fluorophenyl)-4-(2-methyl-1,2,3,6-tetrahydropyridin-4-yl)-3-(pyridin-4-yl)-1H-pyrrole 321344-25-6P, 2-(4-Fluorophenyl)-4-(2-methylpiperidin-4-yl)-3-(pyridin-4-321344-27-8P, 4-(1-Ethylpiperidin-4-yl)-2-(4yl)-1H-pyrrole fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole 321344-29-0P, 2-(4-Fluorophenyl)-4-(1-isopropylpiperidin-4-yl)-3-(pyridin-4-yl)-1H-321344-30-3P, 2-(4-Fluorophenyl)-4-(1-propyl-1,2,3,6tetrahydropyridin-4-yl)-3-(pyridin-4-yl)-1H-pyrrole 321344-31-4P, 4-(1-Benzyl-1,2,3,6-tetrahydropyridin-4-yl)-2-(4-fluorophenyl)-3-(pyridin-321344-32-5P, 2-(4-Fluorophenyl)-4-(1-phenethyl-1,2,3,6-4-yl)-1H-pyrrole tetrahydropyridin-4-yl)-3-(pyridin-4-yl)-1H-pyrrole 321344-35-8P, 4-(1,6-Dimethyl-1,2,3,6-tetrahydropyridin-4-yl)-2-(4-fluorophenyl)-3-321344-36-9P, 4-(1,2-Dimethyl-1,2,3,6-(pyridin-4-yl)-1H-pyrrole tetrahydropyridin-4-yl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole 321344-38-1P, 2-(4-Fluorophenyl)-4-(1,2,2,6,6-pentamethylpiperidin-4-yl)-3-321344-39-2P, 2-(4-Fluorophenyl)-3-(pyridin-4-(pyridin-4-yl)-1H-pyrrole $y\overline{1}$) -4-(1,2,3,6-tetrahydropyridin-5-yl) -1H-pyrrole 321344-41-6P, 4-(4-Aminobutyl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole 321344-42-7P, 1-(2-Dimethylaminoethyl)-3-(4-fluorophenyl)-2-(pyridin-4-yl)-321344-43-8P, 1-(2,2-Dimethyl-3-dimethylaminopropyl)-3-(4-1H-pyrrole fluorophenyl) -2-(pyridin-4-yl) -1H-pyrrole 321344-44-9P, 1-(8-Azabicyclo[3.2.1]octan-3-yl)-3-(4-fluorophenyl)-2-(pyridin-4-yl)-1H-321344-45-0P, 3-(4-Fluorophenyl)-1-(2-methylpiperidin-4-yl)-2-321344-46-1P, 3-(4-Fluorophenyl)-2-(2-(pyridin-4-yl)-1H-pyrrole methylaminopyridin-4-yl)-1-(piperidin-4-yl)-1H-pyrrole 321344-47-2P, 2-(4-Fluorophenyl)-3-[2-((1S)-1-phenylethylamino)pyridin-4-yl]-4-(1,2,3,6-321344-48-3P, 4-(1-tert-Butyl-1,2,3,6tetrahydropyridin-4-yl)-1H-pyrrole tetrahydropyridin-4-yl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole 321344-49-4P, 2-(4-Fluorophenyl)-4-(1-octyl-1,2,3,6-tetrahydropyridin-4yl)-3-(pyridin-4-yl)-1H-pyrrole 321344-50-7P, 4-(1-Ethyl-6-methyl-1,2,3,6-tetrahydropyridin-4-yl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-321344-51-8P, 4-(1-Ethyl-2-methyl-1,2,3,6-tetrahydropyridin-4yl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole 321344-52-9P, 2-(4-Fluorophenyl)-4-(1,2,3,5,6,7,8,8a-octahydroindolizin-7-yl)-3-(pyridin-321344-53-0P, 4-(6-Allyl-1-methyl-1,2,3,6-4-yl)-lH-pyrrole tetrahydropyridin-4-yl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole 321344-54-1P, 4-(2-Allyl-1-methyl-1,2,3,6-tetrahydropyridin-4-yl)-2-(4-methyl-1,2,3,6-tetrahydropyridin-4-321344-55-2P, fluorophenyl) -3-(pyridin-4-yl)-1H-pyrrole 4-(6-Benzyl-1-methyl-1,2,3,6-tetrahydropyridin-4-yl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole 321344-56-3P, 4-(2-Benzyl-1-methyl-1,2,3,6tetrahydropyridin-4-yl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole 321344-59-6P, 2-(4-Fluorophenyl)-4-(6-methyl-1-propyl-1,2,3,6-321344-61-0P, tetrahydropyridin-4-yl)-3-(pyridin-4-yl)-1H-pyrrole 2-(4-Fluorophenyl)-4-(2-methyl-1-propyl-1,2,3,6-tetrahydropyridin-4-yl)-3-321344-62-1P, 2-(4-Fluorophenyl)-4-(pyridin-4-yl)-1H-pyrrole (1,3,4,6,7,9a-hexahydro-2H-quinolizin-8-yl)-3-(pyridin-4-yl)-1H-pyrrole 321344-63-2P, 2-(4-Fluorophenyl)-4-(1,3,4,6,9,9a-hexahydro-2H-quinolizin-8-321344-64-3P, 2-(4-Fluorophenyl)-4yl) -3-(pyridin-4-yl) -1H-pyrrole (1,2,3,5,8,8a-hexahydroindolizin-7-yl)-3-(2-methylaminopyrimidin-4-yl)-1H-321344-65-4P, 2-(4-Fluorophenyl)-4-(1,2,3,5,6,8ahexahydroindolizin-7-yl)-3-(2-methylaminopyrimidin-4-yl)-1H-pyrrole 321344-66-5P, 2-(3,4-Difluorophenyl)-4-(1,2,3,5,8,8a-hexahydroindolizin-7yl)-3-(pyridin-4-yl)-1H-pyrrole 321344-67-6P, 2-(3,4-Difluorophenyl)-4-(1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole 321344-68-7P, 4-(1,2,3,5,8,8a-Hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-2-(3-trifluoromethylphenyl)-1H-pyrrole 321344-69-8P, 4-(1,2,3,5,6,8a-Hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-2-(3-trifluoromethylphenyl)-1H-

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321344-70-1P, 2-(3-Fluorophenyl)-4-(1,2,3,5,8,8a-
pyrrole
hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole
                                                     321344-71-2P,
2-(3-Fluorophenyl)-4-(1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-
                 321344-72-3P, 2-(3-Chlorophenyl)-4-(1,2,3,5,8,8a-
yl)-1H-pyrrole
hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole 321344-73-4P,
2-(3-Chlorophenyl)-4-(1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-
                 321344-74-5P, 4-(1,2,3,5,8,8a-Hexahydroindolizin-7-yl)-2-
yl)-1H-pyrrole
                                    321344-75-6P, 4-(1,2,3,5,6,8a-
phenyl-3-(pyridin-4-yl)-1H-pyrrole
Hexahydroindolizin-7-yl)-2-phenyl-3-(pyridin-4-yl)-1H-pyrrole
321344-76-7P, 2-(4-Fluorophenyl)-3-(pyridin-4-yl)-4-(1,2,3,6-
                                                  443912-04-7P,
tetrahydropyridin-4-yl)-1H-pyrrole
                                    443912-03-6P
4-(3-Dimethylamino-1-propen-1-yl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-
                        443982-91-0P
                                       443982-92-1P
                                                       443982-94-3P
          443982-89-6P
pyrrole
               443982-97-6P
                                             443983-02-6P,
443982-95-4P
                              443983-00-4P
2-(4-Fluorophenyl)-3-(pyridin-4-yl)-4-(6,9,9a,10-tetrahydropyrido[1,2-
                                                         443983-09-3P
                         443983-04-8P
                                        443983-07-1P
a]indol-8-yl)-1H-pyrrole
                              443983-17-3P
                                             443983-19-5P
                                                            443983-21-9P
               443983-15-1P
443983-13-9P
                                                            443983-32-2P
                              443983-29-7P
                                             443983-30-0P
443983-22-0P
               443983-26-4P
              443983-34-4P, 4-(2,2-Diphenyl-1,2,3,5,6,8a-
443983-33-3P
hexahydroindolizin-7-yl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole
              443983-37-7P 443983-39-9P
                                             443983-40-2P
                                                            443983-41-3P
443983-35-5P
                              443983-46-8P
                                                            443983-49-1P
               443983-44-6P
                                             443983-48-0P
443983-43-5P
                             443983-54-8P
                                                            443983-61-7P
              443983-52-6P
                                             443983-58-2P
443983-51-5P
              443983-65-1P
                             443983-67-3P
                                             443983-68-4P
                                                            443983-69-5P
443983-64-0P
                                           443983-78-6P
443983-70-8P
               443983-72-0P
                              443983-75-3P
                                                            443983-80-0P
                             443984-43-8P, 2-(3-Fluorophenyl)-4-(2-methyl-
               443983-84-4P
443983-82-2P
1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole
443984-44-9P, 2-(3-Fluorophenyl)-4-(2-phenyl-1,2,3,5,6,8a-
hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole
                                                       443984-45-0P,
2-(3-Fluorophenyl)-4-(2-methoxy-1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-
                            443984-46-1P, 2-(4-Fluorophenyl)-4-(2-methyl-
(pyridin-4-yl)-1H-pyrrole
1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole
443984-47-2P, 2-(4-Fluorophenyl)-4-(2-phenyl-1,2,3,5,6,8a-
hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole
                                                       443984-48-3P,
2-(4-Fluorophenyl)-4-(2-methoxy-1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-
                            443984-49-4P, 2-(3-Chlorophenyl)-4-(2-methyl-
(pyridin-4-yl)-1H-pyrrole
1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole
443984-50-7P, 2-(3-Chlorophenyl)-4-(2-phenyl-1,2,3,5,6,8a-
                                                       443984-51-8P,
hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole
4-(2-Methyl-1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-2-(3-
                                   443984-52-9P, 4-(2-Phenyl-1,2,3,5,6,8a-
trifluoromethylphenyl)-1H-pyrrole
hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-2-(3-trifluoromethylphenyl)-1H-
          443984-53-0P, 4-(2-Methoxy-1,2,3,5,6,8a-hexahydroindolizin-7-y1)-
3-(pyridin-4-yl)-2-(3-trifluoromethylphenyl)-1H-pyrrole
                                                          443984-54-1P,
2-(4-Fluorophenyl)-4-(2-methyl-3,5,6,8a-tetrahydroindolizin-7-yl)-3-
                            443984-55-2P, 2-(4-Fluorophenyl)-4-(2-
(pyridin-4-yl)-1H-pyrrole
methylidene-1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-
          443984-56-3P, 4-(2-Ethyl-1,2,3,5,6,8a-hexahydroindolizin-7-yl)-2-
(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole 443984-57-4P,
4-(2-Ethyl-1,2,3,5,6,8a-hexahydroindolizin-7-yl)-2-(3-fluorophenyl)-3-
                            443984-58-5P, 2-(3-Chlorophenyl)-4-(2-ethyl-
(pyridin-4-yl)-1H-pyrrole
1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole
443984-59-6P, 4-(2-Ethyl-1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-(pyridin-
4-yl)-2-(3-trifluoromethylphenyl)-1H-pyrrole
                                               443984-60-9P,
2-(4-Fluorophenyl)-4-(2-propyl-1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-
                            443984-61-0P, 2-(3-Fluorophenyl)-4-(2-propyl-
(pyridin-4-yl)-1H-pyrrole
1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole
443984-62-1P, 2-(3-Chlorophenyl)-4-(2-propyl-1,2,3,5,6,8a-
hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole
                                                       443984-63-2P,
4-(2-Propyl-1,2,3,5,6,8a-hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-2-(3-
trifluoromethylphenyl)-1H-pyrrole
                                   443984-64-3P, 4-(2-Ethyl-3,5,6,8a-
tetrahydroindolizin-7-yl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole
443984-65-4P, 2-(4-Fluorophenyl)-4-(2-propyl-3,5,6,8a-tetrahydroindolizin-
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443984-66-5P, 2-(4-Fluorophenyl)-4-(2-
     7-vl)-3-(pyridin-4-yl)-1H-pyrrole
    phenyl-3,5,6,8a-tetrahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole
     443984-68-7P, 2-(4-Fluorophenyl)-3-(Pyridin-4-yl)-4-(6,7,9a,10-
                                                   471864-21-8P
     tetrahydropyrido[1,2-a]indol-8-yl)-1H-pyrrole
                                  670274-00-7P, 4-(1,2,3,5,6,8a-
                    476487-13-5P
     476487-12-4P
     Hexahydroindolizin-7-yl)-2-phenyl-3-(pyrazin-4-yl)-1H-pyrrole
     670274-08-5P, 2-(3-Chlorophenyl)-4-(2-methoxy-1,2,3,5,6,8a-
     hexahydroindolizin-7-yl)-3-(pyridin-4-yl)-1H-pyrrole
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
        (preparation of heteroaryl-substituted pyrrole derivs. that inhibit
production
       of TNF\alpha)
                                               105-36-2, Ethyl bromoacetate
     78-94-4, Methyl vinyl ketone, reactions
IT
     108-00-9, 2-Dimethylaminoethylamine 109-01-3, 1-Methylpiperazine
                                          109-65-9, Butyl bromide
                                                                      110-89-4,
     109-55-7, 3-Dimethylaminopropylamine
     Piperidine, reactions
                            110-91-8, Morpholine, reactions
                                                               123-00-2,
                                                                      123-90-0,
                                 123-75-1, Pyrrolidine, reactions
     4-(3-Aminopropyl)morpholine
                     501-53-1, Benzyl chloroformate
                                                      532-24-1,
     Thiomorpholine
     8-Methyl-8-azabicyclo[3.2.1]octan-3-one 700-16-3, Pentafluoropyridine
     826-36-8, 2,2,6,6-Tetramethylpiperidin-4-one
                                                  867-13-0, Ethyl
                                                           1074-68-6,
     diethylphosphonoacetate
                              872-85-5, 4-Formylpyridine
                                      1445-73-4, 1-Methylpiperidin-4-one
     4-Formyl-2-methylthiopyrimidine
     1449-46-3, Benzyltriphenylphosphonium bromide
                                                    1465-76-5,
                                 2032-35-1, Bromoacetaldehyde diethyl acetal
     1-tert-Butylpiperidin-4-one
     2407-99-0, 1,2,3,5,6,7,8,8a-Octahydroindolizin-7-one
                                                            2537-48-6,
                                    2627-86-3, (S)-1-Phenylethylamine
     Diethylphosphonoacetonitrile
     2759-28-6, 1-Benzylpiperazine
                                    3612-18-8, 1-Ethylpiperidin-4-one
     3612-20-2, 1-Benzylpiperidin-4-one
                                          3731-38-2, Quinuclidin-3-one
     4124-41-8, p-Toluenesulfonic anhydride
                                              4254-02-8,
     Cyclopentanecarbonitrile
                               5355-68-0, 1-Isopropylpiperidin-4-one
     5554-54-1, 1,2,2,6,6-Pentamethylpiperidin-4-one
                                                      6238-14-8,
                          13669-32-4, 1,2-Dimethylpiperidin-4-one
     3-Aminoquinuclidine
     16217-15-5, (S)-1-Benzyloxycarbonyl-4-oxoproline methyl ester
                                                                     16217-17-7
     16728-64-6, 3-Benzyloxypropylamine 18942-89-7, 2-Nitroethyl acetate
     21823-56-3, 2-Benzyl-1-methylpiperidin-4-one
                                                   23133-37-1,
     1-Propylpiperidin-4-one
                             23581-42-2, Octahydro-2H-quinolizin-2-one
                                              24654-55-5, 3-(4-
     24489-96-1, Ethyl 3-(4-pyridyl)acrylate
     Fluorophenyl)acrolein 28957-72-4, 8-Benzyl-8-azabicyclo[3.2.1]octan-3-
           33329-70-3, 1-Ethoxycarbonyl-1-formylcyclopropane
                                                               36635-66-2
     36768-62-4, 4-Amino-2,2,6,6-tetramethylpiperidine
                                                        37517-81-0, Methyl
                       39742-60-4, 1-Phenethylpiperidin-4-one
                                                                 40114-49-6,
     malonyl chloride
     1-Benzylpiperidin-3-one
                              40432-52-8, 3-Amino-1-(diphenylmethyl)azetidine
     50541-93-0, 4-Amino-1-benzylpiperidine
                                              53369-71-4, 2,2-Dimethyl-3-
                              64187-48-0, (2S,4R)-1-Benzyloxycarbonyl-4-
     dimethylaminopropylamine
     hydroxypyrrolidin-2-carboxylic acid methyl ester
                                                        71072-32-7,
     1-Octylpiperidin-4-one 72180-27-9, (2S)-1-Benzyloxycarbonyl-4,4-
                                    79538-29-7, 2,4,6-Trifluorobenzoyl chloride
     difluoroproline
                      75776-70-4
     96522-37-1, (2S,4R)-1-Benzyloxycarbonyl-4-methoxypyrrolidin-2-carboxylic
            96901-92-7, 3-Amino-8-benzyl-8-azabicyclo[3.2.1]octane
                  115031-85-1, 2,2-Diphenyl-1,2,3,5,6,7,8,8a-
     113490-82-7
     octahydroindolizin-7-one 131747-69-8, 2-Fluoropyridine-4-carboxaldehyde
     135829-03-7, Methyl 1-benzyloxycarbonylindoline-2-carboxylate
     144222-22-0, 4-Aminomethyl-1-(tert-butoxycarbonyl)piperidine
     153290-87-0, (2S,4R)-1-Benzyloxycarbonyl-4-ethoxypyrrolidin-2-carboxylic
            156088-46-9, (S)-4,4-Dimethyl-2-hydroxymethyl-5-oxopyrrolidine
     162167-97-7, 3-Aminomethyl-1-(tert-butoxycarbonyl)piperidine
     165806-95-1, \alpha-(p-Toluenesulfonyl)-4-fluorobenzylisonitrile
     184637-48-7, 3-Amino-1-(tert-butoxycarbonyl)piperidine
                                                              185212-91-3
     186550-13-0, 3-Amino-1-(tert-butoxycarbonyl)pyrrolidine
                                                              190906-83-3,
     2-Methyl-1-propylpiperidin-4-one 203661-73-8, 1-Benzyl-2-methylpiperidin-
             247570-24-7, cis-4-((tert-Butoxycarbonyl)amino)cyclohexane-1-amine
     4-one
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288620-86-0, (2S,4R)-1-Benzyloxycarbonyl-4-hydroxypiperidin-
     263389-45-3
     2-carboxylic acid benzyl ester 306296-67-3, 1-Allyloxycarbonylpiperidin-4-one 321344-85-8 321345-30-6, 4-Amino-1-benzyl-2-
                        321345-31-7, Ethyl 3-(2-fluoropyridin-4-yl)acrylate
     methylpiperidine
     321345-32-8, 1-Ethyl-2-methylpiperidin-4-one
                                                    321345-33-9,
                                       321345-34-0, Ethyl 3-(2-
     2-Allyl-1-methylpiperidin-4-one
     methylthiopyrimidin-4-yl)acrylate
                                         321345-35-1
                                                        321345-36-2
                   443983-92-4, 2-(3-Ethoxycarbonyl-2-oxopropyl)indoline
     321345-37-3
     443983-94-6, Methyl (S)-1-benzyloxycarbonyl-4-phenyl-3-pyrroline-2-
                   443984-09-6, (2S,4S)-4-Methoxypiperidin-2-carboxylic acid
     carboxylate
                     443984-25-6, (S)-1-(Benzyloxycarbonyl)piperidin-2-
     hydrochloride
                                                  443984-42-7
                                                               670274-03-0
     carboxylic acid ethyl ester
                                   443984-41-6
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (preparation of heteroaryl-substituted pyrrole derivs. that inhibit
production
        of TNF\alpha)
                   135829-04-8P, 1-Benzyloxycarbonylindoline-2-methanol
     16217-18-8P
IT
     165807-04-5P 200184-60-7P, (S)-1-Benzyloxycarbonyl-4-methylideneproline
                    290357-27-6P, 2-(4-Fluorophenyl)-3-(pyridin-4-yl)-1H-
     Methyl Ester
               321344-79-0P, 4-Ethoxycarbonyl-2-(4-fluorophenyl)-3-(pyridin-4-
     pyrrole
     \overline{y1})-1H-pyrrole 321344-80-3P, \overline{2}-(4-Fluorophenyl)-4-hydroxymethyl-3-
     (pyridin-4-yl)-1H-pyrrole 321344-81-4P, 2-(4-Fluorophenyl)-4-formyl-3-
     (pyridin-4-yl)-1H-pyrrole 321344-83-6P, 4-(2-Cyanoethyl)-2-(4-
     fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole 321344-84-7P,
     4-[3-(tert-Butoxycarbonylamino)propyl]-2-(4-fluorophenyl)-3-(pyridin-4-yl)-
                  321344-86-9P, 2-(4-Fluorophenyl)-3-(pyridin-4-yl)-1-
     1H-pyrrole
                                      321344-87-0P, 4-Bromo-2-(4-fluorophenyl)-
     (triisopropylsilyl) -1H-pyrrole
     3-(pyridin-4-yl)-1-triisopropylsilyl-1H-pyrrole
                                                       321344-88-1P,
     [5-(4-Fluorophenyl)-4-(pyridin-4-yl)-1-triisopropylsilyl-1H-pyrrol-3-
                                 321344-89-2P
                                                 321344-90-5P,
     yl](pyridin-4-yl)methanol
     2-(4-Fluorophenyl)-4-(4-hydroxypiperidin-4-yl)-3-(pyridin-4-yl)-1-
                                    321344-92-7P
                                                  321344-93-8P,
     triisopropylsilyl-1H-pyrrole
     1-[1-(tert-Butoxycarbonyl)pyrrolidin-3-yl]-3-(4-fluorophenyl)-2-(pyridin-4-
     yl)-1H-pyrrole 321344-94-9P, 1-(1-(Diphenylmethyl)azetidin-3-yl)-3-(4-
     fluorophenyl) -2-(pyridin-4-yl) -1H-pyrrole
                                                 321344-95-0P,
     1-(3-Benzyloxypropyl)-3-(4-fluorophenyl)-2-(pyridin-4-yl)-1H-pyrrole
     321344-96-1P, 3-(4-Fluorophenyl)-1-(3-hydroxypropyl)-2-(pyridin-4-yl)-1H-
               321344-97-2P, 3-(4-Fluorophenyl)-2-(pyridin-4-yl)-1-[3-(4-
                                              321344-98-3P, 1-(3-Azidopropyl)-3-
     toluenesulfonyloxy)propyl]-1H-pyrrole
     (4-fluorophenyl)-2-(pyridin-4-yl)-1H-pyrrole
                                                    321345-00-0P,
     4-(2-Ethoxycarbonylethyl)-2-(4-fluorophenyl)-3-(pyridin-4-yl)-1H-pyrrole
     321345-01-1P, 2-(4-Fluorophenyl)-4-(3-hydroxypropyl)-3-(pyridin-4-yl)-1H-
               321345-02-2P, 2-(4-Fluorophenyl)-3-(pyridin-4-yl)-4-[3-(4-
                                            321345-03-3P, 2-(4-Fluorophenyl)-4-
     toluenesulfonyloxy)propyl]-1H-pyrrole
     (4-hydroxy-1-methylpiperidin-4-yl)-3-(pyridin-4-yl)-1-triisopropylsilyl-1H-
                               321345-05-5P, 1-(1-Benzylpiperidin-4-yl)-3-(4-
               321345-04-4P
     fluorophenyl)-2-(2-methylthiopyrimidin-4-yl)-1H-pyrrole
                                                                321345-06-6P,
     1-(1-Benzylpiperidin-4-yl)-3-(4-fluorophenyl)-2-(2-
     (methanesulfonyl)pyrimidin-4-yl)-1H-pyrrole
                                                    321345-07-7P,
     1-(1-Benzylpiperidin-4-yl)-3-(4-fluorophenyl)-2-(2-methylaminopyrimidin-4-
                      321345-11-3P, 4-(3-Cyanopropyl)-2-(4-fluorophenyl)-3-
     yl)-1H-pyrrole
     (pyridin-4-yl)-1H-pyrrole 321345-12-4P, 1-(1-Benzylpiperidin-4-yl)-3-(4-
     fluorophenyl)-2-(2-fluoropyridin-4-yl)-1H-pyrrole
                                                         321345-13-5P,
     1-(1-Benzylpiperidin-4-yl)-3-(4-fluorophenyl)-2-(2-methylaminopyridin-4-
                     321345-14-6P, 4-Bromo-2-(4-fluorophenyl)-3-(2-
     yl)-1H-pyrrole
     fluoropyridin-4-yl)-1-triisopropylsilyl-1H-pyrrole
                                                           321345-15-7P
     321345-16-8P, 4-(1-Allyloxycarbonyl-1,2,3,6-tetrahydropyridin-4-yl)-2-(4-
     fluorophenyl) -3-[2-((1S)-phenylethylamino)pyridin-4-yl]-1H-pyrrole
     321345-17-9P, 4-Bromo-2-(4-fluorophenyl)-3-(2-methylaminopyrimidin-4-yl)-1-
                                    321345-18-0P, 2-(4-Fluorophenyl)-3-(2-
     triisopropylsilyl-1H-pyrrole
                                            321345-19-1P, 2-(4-Fluorophenyl)-3-
     methylthiopyrimidin-4-yl)-1H-pyrrole
      (2-(methanesulfonyl)pyrimidin-4-yl)-1H-pyrrole 321345-20-4P,
     2-(4-Fluorophenyl)-3-(2-methylaminopyrimidin-4-yl)-1H-pyrrole
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        (preparation of heteroaryl-substituted pyrrole derivs. that inhibit
production
        of TNF\alpha)
     321344-85-8
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (preparation of heteroaryl-substituted pyrrole derivs. that inhibit
production
        of TNF\alpha)
     321344-85-8 HCAPLUS
     1H-Pyrrole-3-carboxaldehyde, 5-(4-fluorophenyl)-4-(4-pyridinyl)-,
     O-methyloxime (9CI) (CA INDEX NAME)
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Section cross-reference(s): 1, 63

ΤТ

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HCAPLUS COPYRIGHT 2004 ACS on STN
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L87
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     2001:62383
AN
     134:115858
DN
     Entered STN: 26 Jan 2001
ED
     Preparation of heteroaryl-substituted pyrroles having excellent inhibitory
ΉT
     activity against the production of inflammatory cytokines
     Kimura, Tomio; Aoki, Kazumasa; Nakao, Akira; Ushiyama, Shigeru; Shimozato,
TN
     Takaichi; Ohkawa, Nobuyuki
     Sankyo Company Limited, Japan
PA
     Eur. Pat. Appl., 367 pp.
SO
     CODEN: EPXXDW
     Patent
DТ
     English
LA
     ICM C07D401-04
IC
         C07D401-14; C07D453-02; C07D451-02; C07D471-04; C07D455-02;
          A61P011-06; A61P009-10; A61P017-06; A61P029-00; A61K031-4427;
          A61K031-4375
     27-16 (Heterocyclic Compounds (One Hetero Atom))
CC
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	MARPAI 134:1150	٥٥							
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$$R^1$$
 R^2
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 R^3

The title compds. [I; A = pyrrole; R1 = (un)substituted aryl or heteroaryl; R2 = (un)substituted nitrogen-containing heteroaryl; R3 = XR4 (wherein X = a single bond, (un)substituted alkylene, alkenylene, alkynylene; R4 = substituted cycloalkyl, aryl, heterocyclyl, etc.); provided that said substituents R1 and R3 are bonded to the two atoms of said pyrrole ring which are adjacent to the atom of the pyrrole ring to which said substituent R2 is bonded] which have excellent inhibitory activity against the production of inflammatory cytokines such as TNF α (biol. data given) and IL-1 β , and are useful in treating arthritis, were prepared and formulated. E.g., a multi-step synthesis of the pyrrole II was given.

pyrrole heteroaryl prepn formulation inflammatory cytokine prodn inhibition; tumor necrosis factor alpha prodn inhibition pyrrole heteroaryl prepn; TNF alpha prodn inhibition pyrrole heteroaryl prepn; interleukin 1beta prodn inhibition pyrrole heteroaryl prepn; antiarthritic pyrrole heteroaryl prepn formulation

IT Antiarthritics

(preparation of heteroaryl-substituted pyrroles having excellent inhibitory activity against the production of inflammatory cytokines)

IT Interleukin 1β

Tumor necrosis factors

RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)

(preparation of heteroaryl-substituted pyrroles having excellent inhibitory

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activity against the production of inflammatory cytokines)
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IT
     321343-74-2P
                    321343-78-6P
                                   321343-82-2P
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     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT
     (Reactant or reagent); USES (Uses)
        (preparation of heteroaryl-substituted pyrroles having excellent inhibitory
        activity against the production of inflammatory cytokines)
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    RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of heteroaryl-substituted pyrroles having excellent inhibitory
        activity against the production of inflammatory cytokines)
IT
     108-00-9, 2-Dimethylaminoethylamine
                                           109-01-3, 1-Methylpiperazine
                                           110-89-4, Piperidine, reactions
     109-55-7, 3-Dimethylaminopropylamine
     110-91-8, Morpholine, reactions
                                      123-00-2, 4-Morpholinepropanamine
                                532-24-1, 8-Methyl-8-azabicyclo[3.2.1]octan-3-
     123-90-0, Thiomorpholine
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           700-16-3, Pentafluoropyridine
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     Tetramethylpiperidin-4-one
     872-85-5, 4-Formylpyridine
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                       2627-86-3, (S)-1-Phenylethylamine
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     1-Benzylpiperazine
                               3731-38-2, Quinuclidin-3-one
                                                               5355-68-0,
     1-Benzylpiperidin-4-one
                                  5554-54-1, 1,2,2,6,6-Pentamethylpiperidin-4-
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           16728-64-6, 3-Benzyloxypropylamine
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     one
               21823-56-3, 2-Benzyl-1-methylpiperidin-4-one
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     acetate
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     28957-72-4, 8-Benzyl-8-azabicyclo[3.2.1]octan-3-one
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                                          79538-29-7, 2,4,6-Trifluorobenzoyl
     71072-32-7, 1-Octylpiperidin-4-one
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Allyloxycarbonylpiperidin-4-one 321345-30-6, 4-Amino-1-benzyl-2-methylpiperidine 321345-31-7, Ethyl 3-(2-fluoropyridin-4-yl)acrylate 321345-32-8, 1-Ethyl-2-methylpiperidin-4-one 321345-33-9, 2-Allyl-1-methylpiperidin-4-one 321345-34-0, Ethyl 3-(2-methylthiopyrimidin-4-yl)acrylate 321345-35-1 321345-36-2 321345-37-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of heteroaryl-substituted pyrroles having excellent inhibitory activity against the production of inflammatory cytokines)

321344-79-0P 321344-80-3P 321344-81-4P 290357-27-6P IT165807-04-5P 321344-84-7P **321344-85-8P** 321344-82-5P 321344-83-6P 321344-87-0P 321344-88-1P 321344-89-2P 321344-90-5P 321344-86-9P 321344-92-7P 321344-93-8P 321344-94-9P 321344-95-0P 321344-91-6P 321344-97-2P 321344-98-3P 321344-99-4P 321345-00-0P 321344-96-1P 321345-04-4P 321345-05-5P 321345-03-3P 321345-02-2P 321345-01-1P 321345-08-8P 321345-09-9P 321345-10-2P 321345-07-7P 321345-06-6P 321345-14-6P 321345-15-7P 321345-12-4P 321345-13-5P 321345-11-3P 321345-17-9P 321345-18-0P 321345-19-1P 321345-20-4P 321345-16-8P 321345-24-8P 321345~25-9P 321345-22-6P 321345-23-7P 321345-21-5P 321345-29-3P 321422-08-6P 321345-27-1P 321345-28-2P 321345-26-0P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of heteroaryl-substituted pyrroles having excellent inhibitory activity against the production of inflammatory cytokines)

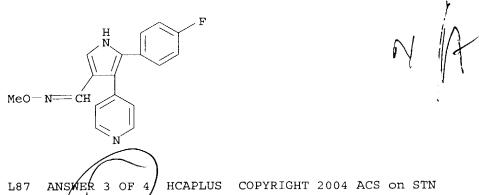
IT 321344-85-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of heteroaryl-substituted pyrroles having excellent inhibitory activity against the production of inflammatory cytokines)

RN 321344-85-8 HCAPLUS

CN 1H-Pyrrole-3-carboxaldehyde, 5-(4-fluorophenyl)-4-(4-pyridinyl)-, O-methyloxime (9CI) (CA INDEX NAME)



AN 1998:473973 /HCAPLUS

DN 129:108993

ED Entered STN: 30 Jul 1998

TI Preparation of pyridylfurans and pyridylthiophenes as inhibitors of $\text{TNF}\alpha$ biosynthesis and CAMs expression.

IN Kawai, Akiyoshi; Kawai, Makoto

PA Pfizer Inc., USA

SO Eur. Pat. Appl., 53 pp. CODEN: EPXXDW

DT Patent

LA English

IC ICM C07D409-04

ICS C07D405-04; C07D493-04; C07D409-14; C07D495-04; A61K031-44

CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1

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                                           JP 1997-366682
                                                             19971226 <--
     JP 10195070
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                                                             19980106 <--
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                                                             19980106 <--
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     JUS 6048880
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                       Α
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     US 6696470
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                                                             20011030 <--
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PRAI WO 1997-IB2
                       W
                                      <---
                            19980106
     US 1998-3108
                       A1
                                      <---
                       B1
                            19990524
     US 1999-317570
     MARPAT 129:108993
os
GΙ
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Title compds. [I; R1, R2 = H, halo, (substituted) (cyclo)alkyl, hydroxy(cyclo)alkyl, alkoxy, alkenyl, alkynyl, (substituted) heterocyclyl, (hetero)aryl, acyl, cyano, NO2, aminocarbonyl, etc.; R3 = (substituted) (cyclo)alkyl, (cyclo)alkylcarbonyl, cyano, formyl, alkenylcarbonyl, alkynylcarbonyl, arylcarbonyl, etc.; R4 = H, halo, alkyl, hydroxyalkyl, alkylcarbonyl, etc.; 2 of R1-R3 = atoms to form (substituted) rings; X = O, S, SO, SO2; m = 0-4; and N-oxides thereof], were prepared Thus, 3-acetyl-2,4-dimethylfuran was refluxed with NBS and AIBN in benzene for 1 h to give 88% 3-acetyl-5-bromo-2,4-dimethylfuran. The latter in dimethoxyethane was refluxed with aqueous NaHCO3 and (Ph3P)2PdCl2 followed by addition of 4-pyridineboronic acid and (Ph3P)2PdCl2 and further reflux to give 31% 3-acetyl-2,4-dimethyl-5-(4-pyridyl)furan. Selected I inhibited TNFα biosynthesis with IC50 = 100 nM to 10 μM.

ST pyridylfuran pyridylthiophene prepn TNF biosynthesis inhibitor; cell adhesion mol expression inhibitor pyridylfuran; drug pyridylfuran pyridylthiophene prepn

IT AIDS (disease)

(-related complex, drugs for; preparation of pyridylfurans and pyridylthiophenes as inhibitors of $\text{TNF}\alpha$ biosynthesis and CAMs expression)

IT Intestine, disease

(Crohn's, treatment; preparation of pyridylfurans and pyridylthiophenes as inhibitors of TNF α biosynthesis and CAMs expression)

IT Antiarteriosclerotics

(antiatherosclerotics; preparation of pyridylfurans and pyridylthiophenes as inhibitors of TNF α biosynthesis and CAMs expression)

IT Tumor necrosis factors

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(biosynthesis inhibitors; preparation of pyridylfurans and pyridylthiophenes as inhibitors of $\text{TNF}\alpha$ biosynthesis and CAMs expression)

IT Malaria Malaria

(cerebral, treatment; preparation of pyridylfurans and pyridylthiophenes as inhibitors of $\text{TNF}\alpha$ biosynthesis and CAMs expression)

IT Intestine, disease

(inflammatory, treatment; preparation of pyridylfurans and pyridylthiophenes as inhibitors of $TNF\alpha$ biosynthesis and CAMs expression)

IT Cell adhesion

(inhibitors; preparation of pyridylfurans and pyridylthiophenes as inhibitors of ${\tt TNF}\alpha$ biosynthesis and CAMs expression)

IT Reperfusion

(injury, treatment; preparation of pyridylfurans and pyridylthiophenes as inhibitors of TNF α biosynthesis and CAMs expression)

IT Brain, disease

Brain, disease

(malaria, treatment; preparation of pyridylfurans and pyridylthiophenes as inhibitors of ${\tt TNF}\alpha$ biosynthesis and CAMs expression)

IT Respiratory distress syndrome

(newborn, treatment; preparation of pyridylfurans and pyridylthiophenes as inhibitors of $\text{TNF}\alpha$ biosynthesis and CAMs expression)

IT Allergy inhibitors

Anti-AIDS agents

Anti-inflammatory agents

Antiarthritics

Antiasthmatics

Anticoagulants

Antidiabetic agents

Antimalarials

Antiobesity agents

Antipyretics

Antitumor agents

Antiviral agents

Cardiovascular agents

(preparation of pyridylfurans and pyridylthiophenes as inhibitors of $\textsc{TNF}\alpha$ biosynthesis and CAMs expression)

IT Bone

(resorption, treatment; preparation of pyridylfurans and pyridylthiophenes as inhibitors of TNF α biosynthesis and CAMs expression)

IT Shock (circulatory collapse)

(septic, treatment; preparation of pyridylfurans and pyridylthiophenes as inhibitors of TNF α biosynthesis and CAMs expression)

IT Shock (circulatory collapse)

(toxic shock syndrome, treatment; preparation of pyridylfurans and pyridylthiophenes as inhibitors of $TNF\alpha$ biosynthesis and CAMs expression)

IT Cachexia

Keloid

Psoriasis

Sepsis

Silicosis

Skin, disease

Transplant rejection

(treatment; preparation of pyridylfurans and pyridylthiophenes as inhibitors of $\text{TNF}\alpha$ biosynthesis and CAMs expression)

IT Intestine, disease

(ulcerative colitis, treatment; preparation of pyridylfurans and pyridylthiophenes as inhibitors of $\text{TNF}\alpha$ biosynthesis and CAMs expression)

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210097-13-5P
                                    210097-28-2P
                                                   210097-33-9P
                                                                   210097-47-5P
IT
     210096-98-3P
     210097-55-5P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT
     (Reactant or reagent); USES (Uses)
        (preparation of pyridylfurans and pyridylthiophenes as inhibitors of
        TNF\alpha biosynthesis and CAMs expression)
                    210096-99-4P
                                    210097-00-0P
                                                   210097-02-2P
                                                                   210097-03-3P
IT
     207307-41-3P
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     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of pyridylfurans and pyridylthiophenes as inhibitors of
        TNF\alpha biosynthesis and CAMs expression)
                                        75-16-1, Methylmagnesium bromide
IΤ
     74-89-5, Methylamine, reactions
     98-80-6, Benzeneboronic acid
                                   103-67-3, N-Methylbenzylamine
                        108-30-5, reactions 108-95-2, Phenol, reactions piperazine 110-89-4, Piperidine, reactions
                                               108-95-2, Phenol, reactions
     Diethyl malonate
     109-01-3, N-Methylpiperazine
                                                                        110-91-8,
                            116-09-6, Hydroxyacetone
                                                         124-40-3,
     Morpholine, reactions
                                367-12-4, 2-Fluorophenol
                                                             371-41-5,
     Dimethylamine, reactions
                                                        562-46-9,
                      504-02-9, 1,3-Cyclohexanedione
     4-Fluorophenol
     4,4-Dimethyl-1,3-Cyclohexanedione
                                         593-56-6, Methoxylamine hydrochloride
     616-44-4, 3-Methylthiophene 638-00-6, 2,4-Dimethylthiophene
     Methyllithium
                     1194-18-9, 1,3-Cycloheptanedione
                                                          1641-09-4,
                                                                   1692-15-5,
                        1679-18-1, 4-Chlorobenzeneboronic acid
     3-Cyanothiophene
     4-Pyridineboronic acid
                              1692-25-7, 3-Pyridineboronic acid
                                                2713-31-7, 2,5-Difluorophenol
     4-Fluorobenzeneboronic acid
                                    1993-03-9
     3172-52-9, 2,5-Dichlorothiophene
                                        4414-45-3
                                                     5077-67-8,
     1-Hydroxy-2-butanone
                            5720-07-0, 4-Methoxybenzeneboronic acid
     6165-69-1, 3-Thiopheneboronic acid 25074-25-3
                                                        30318-99-1,
                                32933-07-6, 3-Acetyl-2,4-dimethylfuran
     3-Bromo-4-methylthiophene
                  36157-40-1, 3-Acetyl-2,5-dichlorothiophene
                                                                 39177-23-6,
     33177-29-6
                                 41903-50-8, Hydroxyacetophenone
                                                                     57248-14-3,
     3-(4-Fluorophenoxy)phenol
     2,5-Dichloro-3-thiophenecarbonyl chloride
                                                  69213-94-1
                                                                69213-95-2
                              128796-39-4, 4-Trifluoromethylbenzeneboronic
                  98546-51-1
     85006-25-3
                                                                      210098-27-4
            145129-54-0
                          207307-53-7
                                         210098-25-2
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     210098-28-5
     210098-34-3
                   210098-36-5
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (preparation of pyridylfurans and pyridylthiophenes as inhibitors of
        {\tt TNF}\alpha biosynthesis and CAMs expression)
                                7687-78-7P
                                             7687-79-8P
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                  7687-77-6P
TT
     6906-61-2P
     17249-90-0P, 2,5-Dichloro-3-methylthiophene
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                                  34967-65-2P
                                                35061-13-3P
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                   33449-56-8P
     32933-05-4P
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                                                63826-68-6P
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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of pyridylfurans and pyridylthiophenes as inhibitors of $TNF\alpha$ biosynthesis and CAMs expression)

RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD RE

- (1) Bacon, E; J HETEROCYCL CHEM 1991, V28(8), P1953 HCAPLUS
- (2) Gilat, S; J CHEM SOC, CHEM COMMUN 1993, 18, P1439 HCAPLUS
- (3) Katritzky, A; ENERGY FUELS 1990, V4(5), P572 HCAPLUS
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- (5) Pfizer Pharma; WO 9802430 A HCAPLUS
- (6) Ribereau, P; C R HEBD SEANCES ACAD SCI, SER C 1975, V280(5), P293 HCAPLUS
- (7) Zhang, Y; J HETEROCYCL CHEM 1993, V30(5), P1293 HCAPLUS
- IT 210097-56-6P 210097-62-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyridylfurans and pyridylthiophenes as inhibitors of $\text{TNF}\alpha$ biosynthesis and CAMs expression)

- RN 210097-56-6 HCAPLUS
- CN 3-Thiophenecarboxaldehyde, 4-methyl-2,5-di-4-pyridinyl-, 0-acetyloxime (9CI) (CA INDEX NAME)

RN 210097-62-4 HCAPLUS

CN 3-Thiophenecarboxaldehyde, 4-methyl-2,5-di-4-pyridinyl-, 0-methyloxime, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

L87 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

- AN 1993: 51800 HCAPLUS
- DN 118:51800
- ED Entered STN: 16 Feb 1993
- Oxidation of carbovir, a carbocyclic nucleoside, by rat liver cytosolic enzymes. Enantioselectivity and enantiomeric inhibition
- AU Patanella, James E.; Walsh, John S.

```
Res. Inst., Glaxo, Inc., Research Triangle Park, NC, USA
CS
    Drug Metabolism and Disposition (1992), 20(6), 912-19
SO
     CODEN: DMDSAI; ISSN: 0090-9556
DT
     Journal
     English
LA
     1-2 (Pharmacology)
CC
     Previous metabolism studies of (-)-cis-carbovir (1'R-cis-2-amino-1,9-dihydro-9-
ĀΒ
     [4'S-hydroxymethyl-2-cyclopenten-1-yl]-6H-purin-6-one), an
     antiviral agent, have shown that the major route of metabolism of
     carbovir in the rat is oxidation of the methylene hydroxyl group of the
     cyclopentadiene ring to form the corresponding 4'-carboxylic acid
     metabolite. We have determined that rat hepatic alc. dehydrogenase and
     aldehyde dehydrogenase are responsible for this biotransformation through
     sequential oxidation of the alc. through the aldehyde to the carboxylic acid.
     The results of incubations of racemic (\pm)-cis-carbovir with rat liver
     cytosol showed that this oxidation occurs enantioselectively favoring the
     (+)-enantiomer by a factor of 6- to 7-fold. We have proven that alc.
     dehydrogenase contributes to the enantioselectivity of the overall oxidation
     process, but were unable to determine whether or not any contribution is made
     by aldehyde dehydrogenase. Parallel incubations conducted with the sep.
     enantiomers revealed that the concentration required to achieve a half-maximal
     rate for the oxidation of the (+)-enantiomer (0.27 mM) was one-fifth that
     required for the (-)-enantiomer (1.36 mM). Results from enantiomeric
     inhibition studies showed that (+)-carbovir inhibited the oxidation of
     (-)-carbovir. In contrast, (-)-carbovir did not inhibit the oxidation of
     (+)-carbovir.
     carbovir oxidn liver
ST
IT
     Liver, metabolism
        (carbovir metabolism in, enantioselectivity and enantiomeric inhibition in)
     9028-86-8, Aldehyde dehydrogenase
TT
     RL: BIOL (Biological study)
        (carbovir aldehyde intermediate oxidation by, enantioselectivity of)
     9031-72-5, Alcohol dehydrogenase
IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (carbovir oxidation by, enantioselectivity of)
                   132012-22-7 145414-80-8 145414-81-9
     131956-47-3
IT
     RL: FORM (Formation, nonpreparative)
        (formation of, as carbovir conjugative metabolite, enantioselectivity
        and enantiomeric inhibition in)
     145414-78-4
TT
     RL: FORM (Formation, nonpreparative)
        (formation of, as carbovir oxidative metabolite, enantioselectivity and
        enantiomeric inhibition in)
     118353-05-2
IT
     RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL
     (Biological study); PROC (Process)
        (metabolism of, in liver, enantioselectivity and enantiomeric inhibition
        in)
                                124915-24-8, (+)-Carbovir
     120443-30-3, (-)-Carbovir
IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (oxidation of, by alc. dehydrogenase, enantioselectivity in)
TT
     145356-37-2P 145414-79-5P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of, as carbovir aldehyde intermediate trap)
     145414-80-8 145414-81-9
IT
     RL: FORM (Formation, nonpreparative)
        (formation of, as carbovir conjugative metabolite, enantioselectivity
        and enantiomeric inhibition in)
     145414-80-8 HCAPLUS
RN
     2-Cyclopentene-1-carboxaldehyde, 4-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-
     yl)-, 1-(O-methyloxime), [1R-[1\alpha(E),4\alpha]]- (9CI) (CA INDEX
     NAME)
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RN 145414-81-9 HCAPLUS

CN 2-Cyclopentene-1-carboxaldehyde, 4-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)-, 1-(0-methyloxime), [1R-[1 α (Z),4 α]]- (9CI) (CA INDEX NAME)

IT 145356-37-2P 145414-79-5P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as carbovir aldehyde intermediate trap)

RN 145356-37-2 HCAPLUS

2-Cyclopentene-1-carboxaldehyde, 4-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)-, 1-(0-methyloxime), [1S-[1α(Σ),4α]]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ H_2N & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ \end{array}$$

RN 145414-79-5 HCAPLUS

CN 2-Cyclopentene-1-carboxaldehyde, 4-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)-, 1-(0-methyloxime), [1S-[1 α (E),4 α]- (9CI) (CA INDEX NAME)